

Kernel Methods in Machine Learning

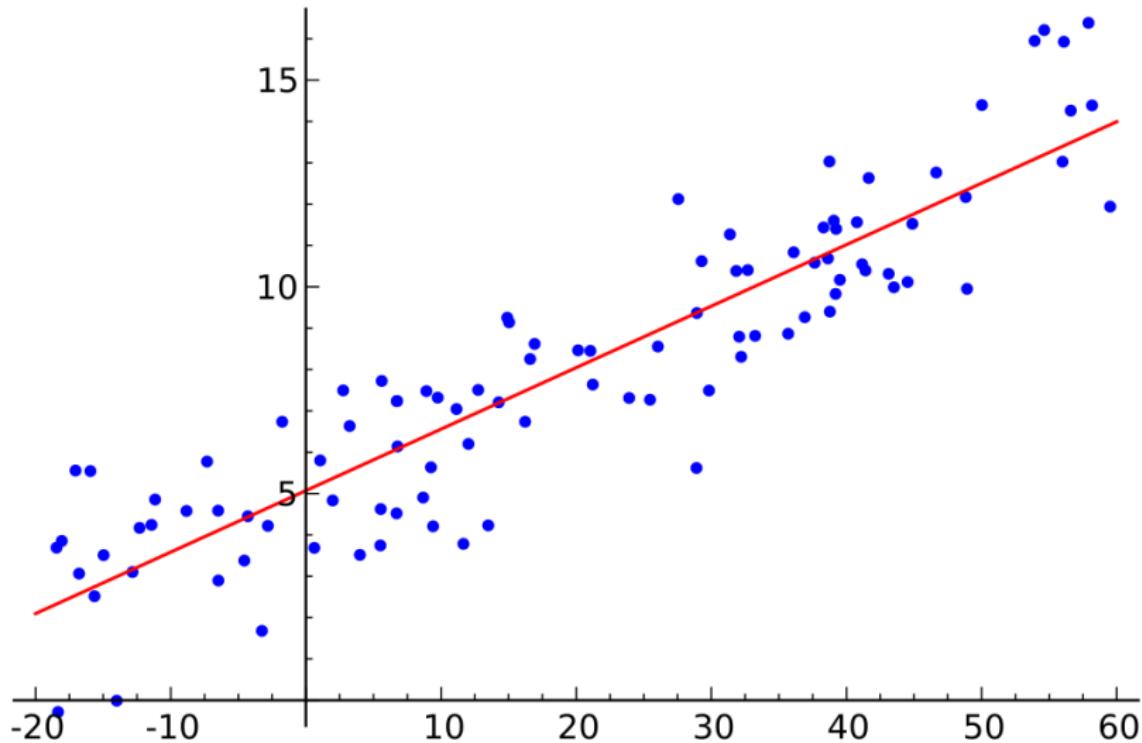
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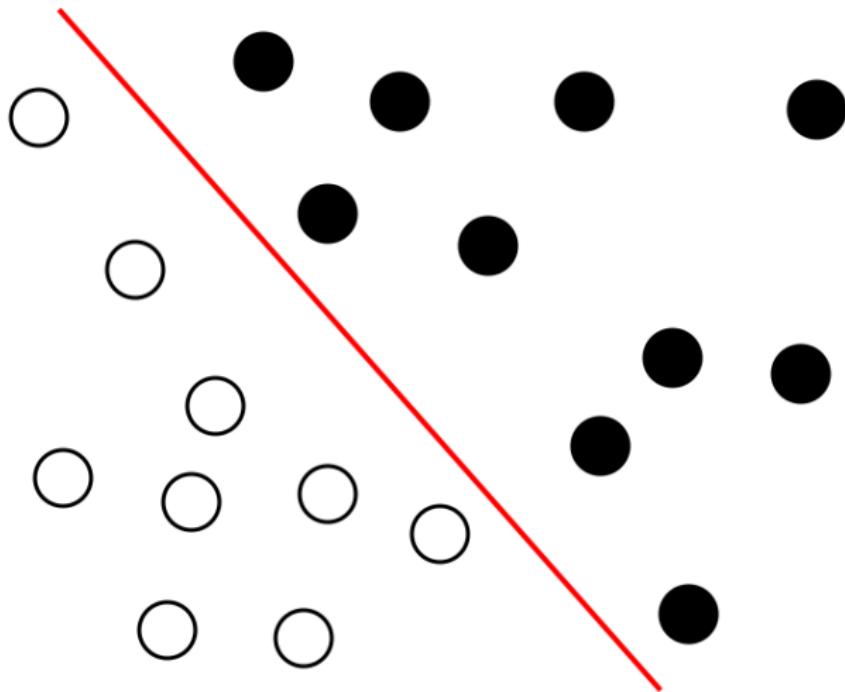
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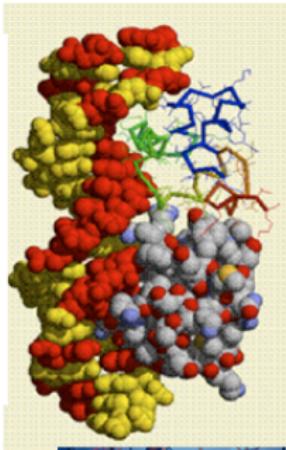
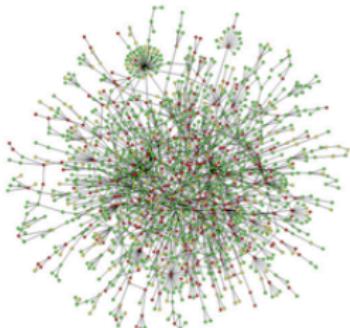
What we know how to solve



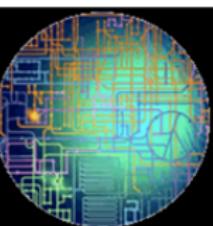
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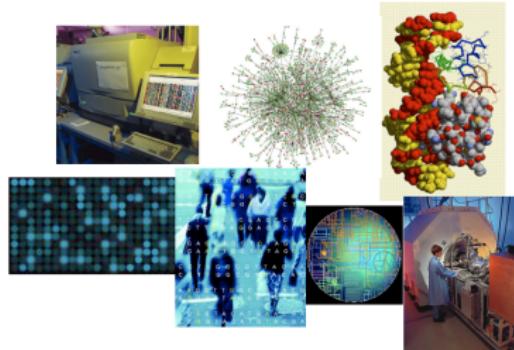
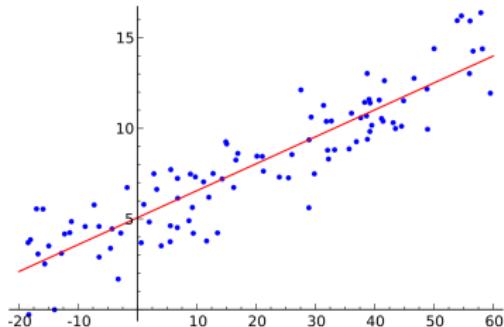
But real data are often more complicated...



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C C T T G G G C G T T A C A A
C A T T T G G C G T T A C A C
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Main goal of this course



Extend
well-understood, linear statistical learning techniques
to
real-world, complicated, structured, high-dimensional data
based on
a rigorous mathematical framework
leading to
practical modelling tools and algorithms

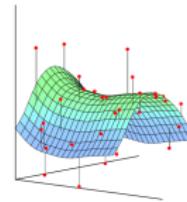
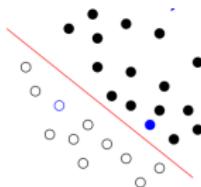
Outline

- 1 Learning in high dimension
- 2 Learning with ℓ_2 regularization
 - Ridge regression
 - Ridge logistic regression
 - Linear hard-margin SVM
 - Interlude: quick notes on constrained optimization
 - Back to hard-margin SVM
 - Soft-margin SVM
 - Large-margin classifiers
- 3 Learning with kernels
 - Kernel methods
 - Positive definite kernels and RKHS
 - Kernel examples
 - Multiple Kernel Learning (MKL)
- 4 Conclusion

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General learning framework



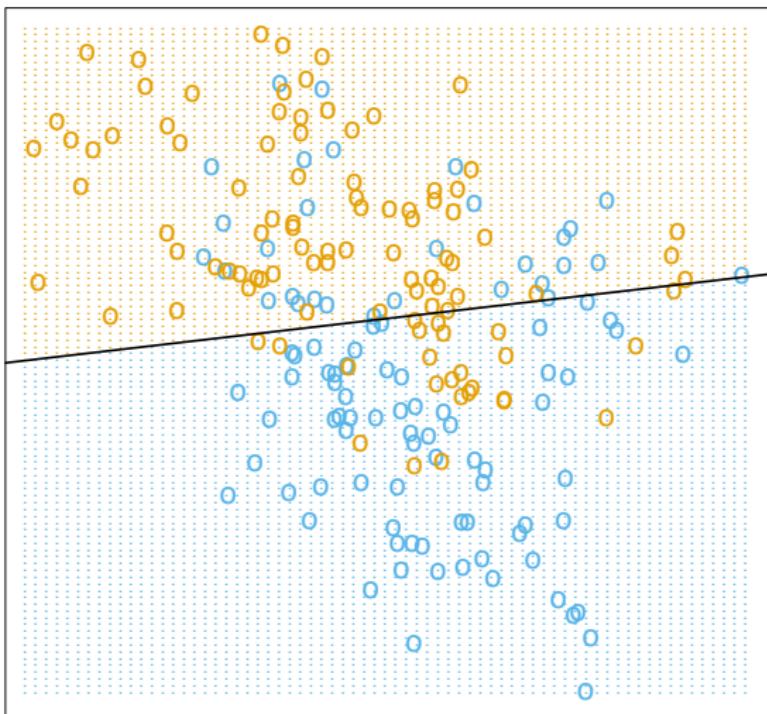
Input

- \mathcal{X} the space of **patterns** or **data** (typically, $\mathcal{X} = \mathbb{R}^p$)
- \mathcal{Y} the space of **response** or **labels**
 - Classification or pattern recognition : $\mathcal{Y} = \{-1, 1\}$
 - Regression : $\mathcal{Y} = \mathbb{R}$
 - Structured output: \mathcal{Y} general
- $\mathcal{S} = \{(x_1, y_1), \dots, (x_n, y_n)\}$ a **training set** in $(\mathcal{X} \times \mathcal{Y})^n$

Output

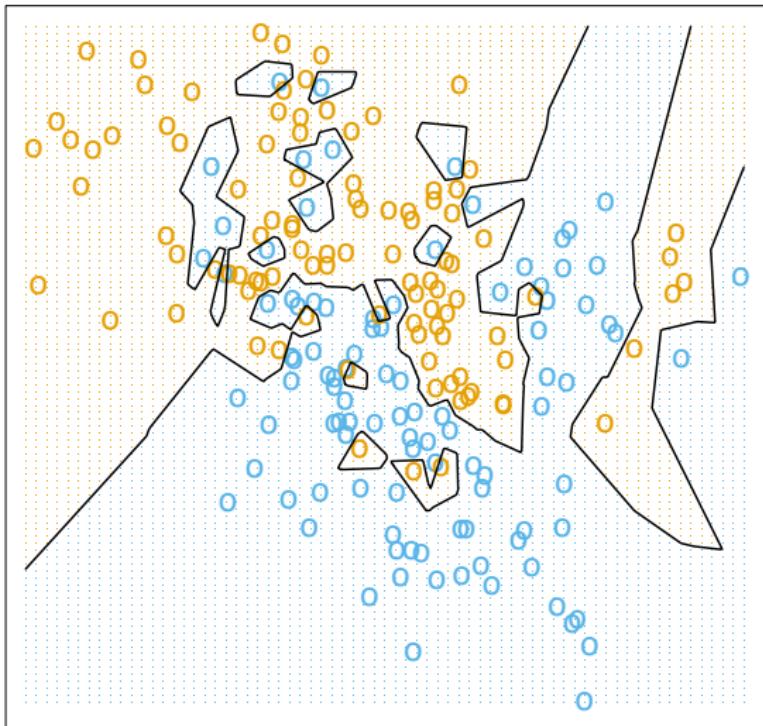
- A **function** $f : \mathcal{X} \rightarrow \mathcal{Y}$ to predict the output associated to any new pattern $x \in \mathcal{X}$ by $f(x)$

Simple example 1 : ordinary least squares (OLS)



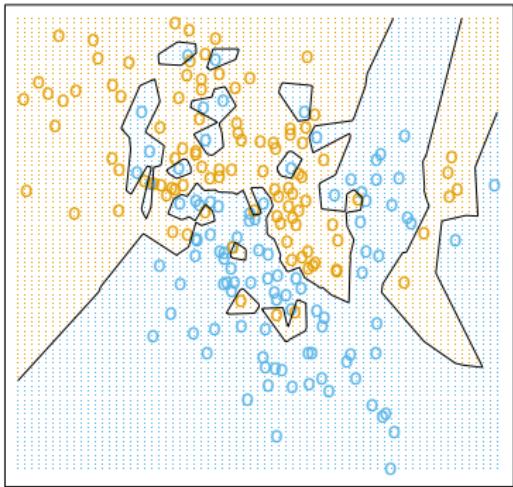
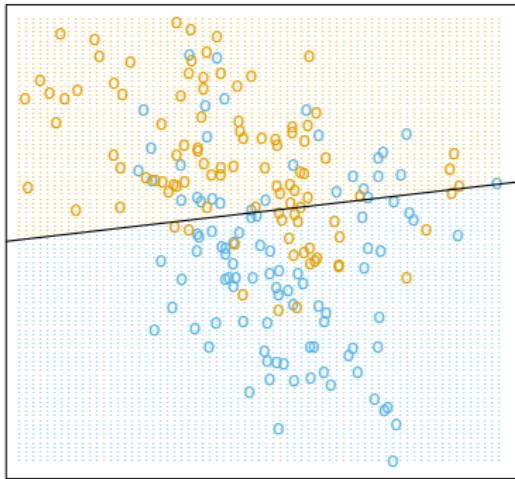
(Hastie et al. *The elements of statistical learning*. Springer, 2001.)

Simple example 2 : 1-nearest neighbor (1-NN)



(Hastie et al. *The elements of statistical learning*. Springer, 2001.)

What's wrong?



- OLS: the linear separation is not appropriate = "large bias"
- 1-NN: the classifier seems too unstable = "large variance"

The fundamental "bias-variance" trade-off

- Assume $Y = f(X) + \epsilon$, where ϵ is some noise
- From the training set \mathcal{S} we estimate the predictor \hat{f}
- On a new point x_0 , we predict $\hat{f}(x_0)$ but the "true" observation will be $Y_0 = f(x_0) + \epsilon$
- On average, we make an error of:

$$\begin{aligned} & E_{\epsilon, \mathcal{S}} \left(Y_0 - \hat{f}(x_0) \right)^2 \\ &= E_{\epsilon, \mathcal{S}} \left(f(x_0) + \epsilon - \hat{f}(x_0) \right)^2 \\ &= E\epsilon^2 + E_{\mathcal{S}} \left(f(x_0) - \hat{f}(x_0) \right)^2 \\ &= E\epsilon^2 + \left(f(x_0) - E_{\mathcal{S}} \hat{f}(x_0) \right)^2 + E_{\mathcal{S}} \left(\hat{f}(x_0) - E_{\mathcal{S}} \hat{f}(x_0) \right)^2 \\ &= \text{noise} + \text{bias}^2 + \text{variance} \end{aligned}$$

Important message

Future prediction error = noise + bias² + variance

- The "noise" part can not be avoided
- By choosing a learning model, we should consider both "bias" and "variance" if we want to make good predictions
- Intuitively, a **more realistic, more complex model** with more parameters to estimate has **smaller bias but larger variance**
- If variance dominates bias (eg, in high dimension), then having more complex, more realistic models can hurt performance
- In other words, **a wrong but simple model can work better than a more realistic but more complex model**
- In many applications, domain experts (non-statisticians) often ignore the cost of complexity and prefer complex models, which can lead to disappointing results. You can help them!

Back to OLS

- Linear model with parameter $\beta \in \mathbb{R}^p$:

$$\forall x \in \mathbb{R}^p, \quad f_\beta(x) = \beta^\top x \quad \left(= \sum_{i=1}^p \beta_i x_i \right)$$

- Estimate $\hat{\beta}^{OLS}$ from training data to minimize the mean sum of squares (MSE):

$$\text{MSE}(\beta) = \frac{1}{n} \sum_{i=1}^n (y_i - f_\beta(x_i))^2$$

Back to OLS (cont.)

- Let's use matrix notations:

- $Y = (y_1, \dots, y_n)^\top \in \mathbb{R}^n$ the vector of outcomes
- $X = (x_1, \dots, x_n)^\top \in \mathbb{R}^{n \times p}$ the matrix (n rows=samples, p columns=features)

- We can rewrite MSE as

$$\text{MSE}(\beta) = \frac{1}{n} (Y - X\beta)^\top (Y - X\beta)$$

- $\text{MSE}(\beta)$ is a quadratic convex function; we minimize it by setting its gradient to 0:

$$\nabla_\beta \text{MSE}(\beta) = \frac{2}{n} X^\top (X\beta - Y) = 0$$

- If $X^\top X$ is non-singular, the minimum is reached at

$$\hat{\beta}^{OLS} = \underset{\beta}{\operatorname{argmin}} \text{MSE}(\beta) = (X^\top X)^{-1} X^\top Y$$

Properties of OLS

Bias and variance of OLS

- Assume $Y = X\beta^* + \epsilon$, where $E\epsilon = 0$ and $E\epsilon\epsilon^\top = \sigma^2 I$.
- Then the least squares estimator

$$\hat{\beta}^{OLS} = (X^\top X)^{-1} X^\top Y$$

satisfies

$$\begin{cases} E(\hat{\beta}^{OLS}) = \beta^*, \\ Var(\hat{\beta}^{OLS}) = E(\hat{\beta}^{OLS} - \beta^*)(\hat{\beta}^{OLS} - \beta^*)^\top = \sigma^2 (X^\top X)^{-1}. \end{cases}$$

Proof: exercice

Optimality of OLS

Gauss-Markov theorem

- Assume $Y = X\beta^* + \epsilon$, where $E\epsilon = 0$ and $E\epsilon\epsilon^\top = \sigma^2 I$.
- Then the least squares estimator $\hat{\beta}^{OLS}$ is **BLUE** (best linear unbiased estimator), i.e., for any other estimator $\tilde{\beta} = CY$ with $E\tilde{\beta} = \beta^*$,

$$\text{Var}(\hat{\beta}^{OLS}) \preccurlyeq \text{Var}(\tilde{\beta}) \quad \left(\Leftrightarrow \forall x_0, \text{Var}(x_0^\top \hat{\beta}^{OLS}) \leq \text{Var}(x_0^\top \tilde{\beta}) \right)$$

Proof: exercice

- For $\tilde{\beta} = CY$, define $D = C - (X^\top X)^{-1}X^\top$
- Show that if $\tilde{\beta}$ is unbiased, then $DX = 0$
- Show that $\text{Var}(\tilde{\beta}) = \text{Var}(\hat{\beta}^{OLS}) + \sigma^2 DD^\top$

Is BLUE good enough?

OLS mean prediction variance

Suppose $(x_i, y_i)_{i=0, \dots, n}$ are i.i.d. random pairs that follow a distribution (x, y) with

$$Ex = 0, \quad Exx^\top = C,$$

$$y = x^\top \beta^* + \epsilon, \quad E\epsilon = 0, \quad E\epsilon^2 = 1,$$

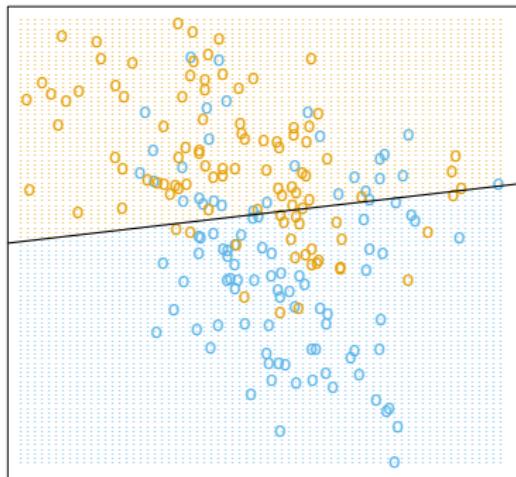
then

$$E_{S, x_0} \text{Var}(f(x_0)) = E_{S, x_0} \text{Var}(x_0^\top \hat{\beta}^{OLS}) = \frac{\sigma^2 p}{n}.$$

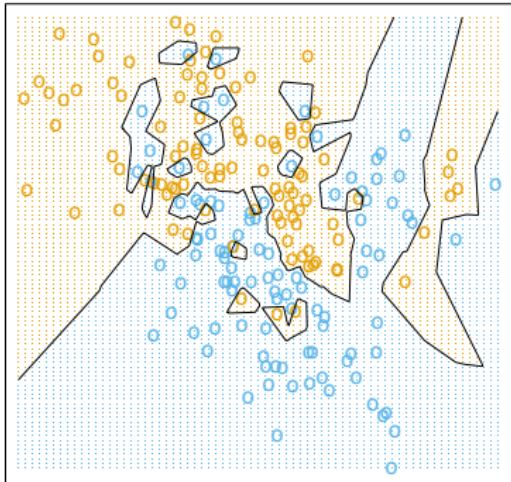
Proof:

$$\begin{aligned} E_{S, x_0} \text{Var}(x_0^\top \hat{\beta}^{OLS}) &= \sigma^2 E_{S, x_0} [x_0^\top (X^\top X)^{-1} x_0] \\ &= \sigma^2 E_{S, x_0} \text{Trace} [(X^\top X)^{-1} x_0 x_0^\top] \\ &= \sigma^2 \text{Trace} [E_S (X^\top X)^{-1} \times E_{x_0} x_0 x_0^\top] \\ &= \sigma^2 \text{Trace} [(nC)^{-1} \times C] \\ &= \sigma^2 p/n \end{aligned}$$

The curse of dimensionality



Small dimension



Large dimension

- In high dimensions, **variance dominates**, even for simple linear estimators.
- **BLUE estimators are therefore useless.**
- In that case, we may have smaller total risk by **increasing bias and decreasing variance**

A solution: shrinkage estimators

- ① Define a large family of "candidate classifiers", e.g., **linear predictors**:

$$f_{\beta}(x) = \beta^T x \quad \text{for } x \in \mathbb{R}^p$$

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- ② For any candidate classifier f_{β} , quantify how "good" it is on the training set with some **empirical risk**, e.g.:

$$R(\beta) = \frac{1}{n} \sum_{i=1}^n (f_{\beta}(x_i) - y_i)^2.$$

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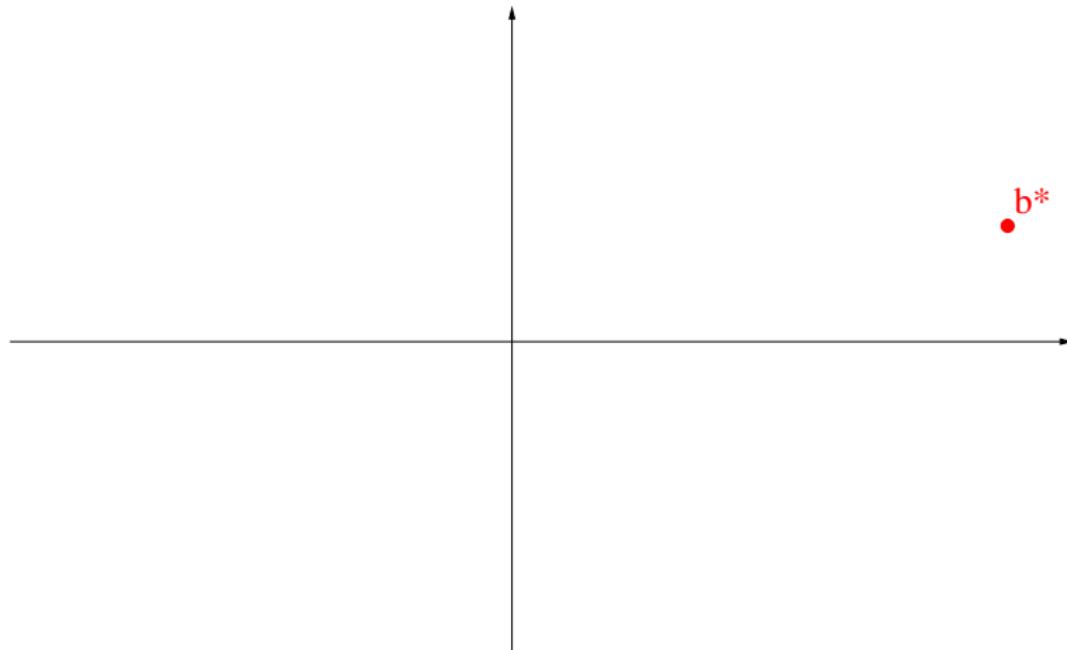
- ③ Choose β that achieves the minimum empirical risk, subject to some **constraint**:

$$\min_{\beta} R(\beta) \quad \text{subject to} \quad \Omega(\beta) \leq C,$$

for some **penalty function** $\Omega : \mathbb{R}^p \rightarrow \mathbb{R}^+$ and $C \geq 0$.

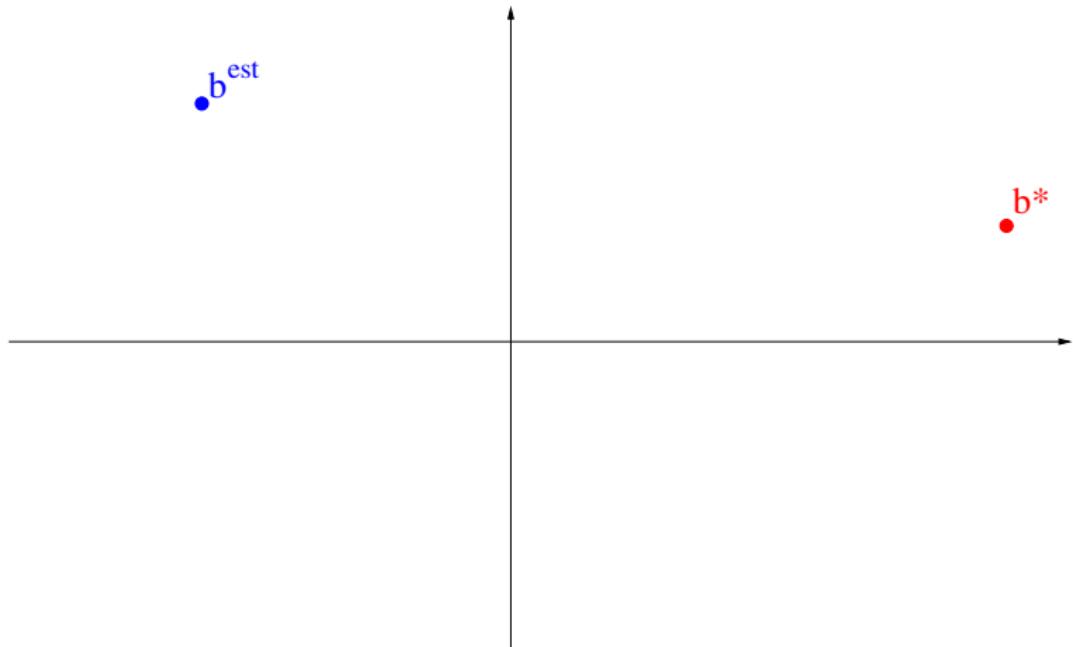
Why skrinkage classifiers?

$$\min_{\beta} R(\beta) \quad \text{subject to} \quad \Omega(\beta) \leq C .$$



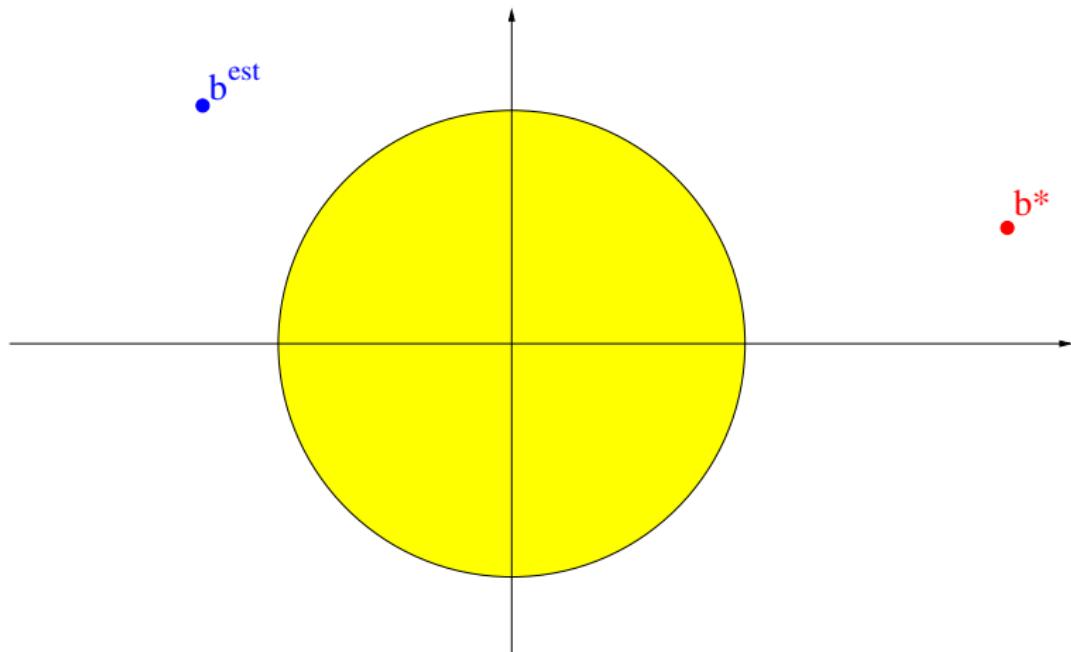
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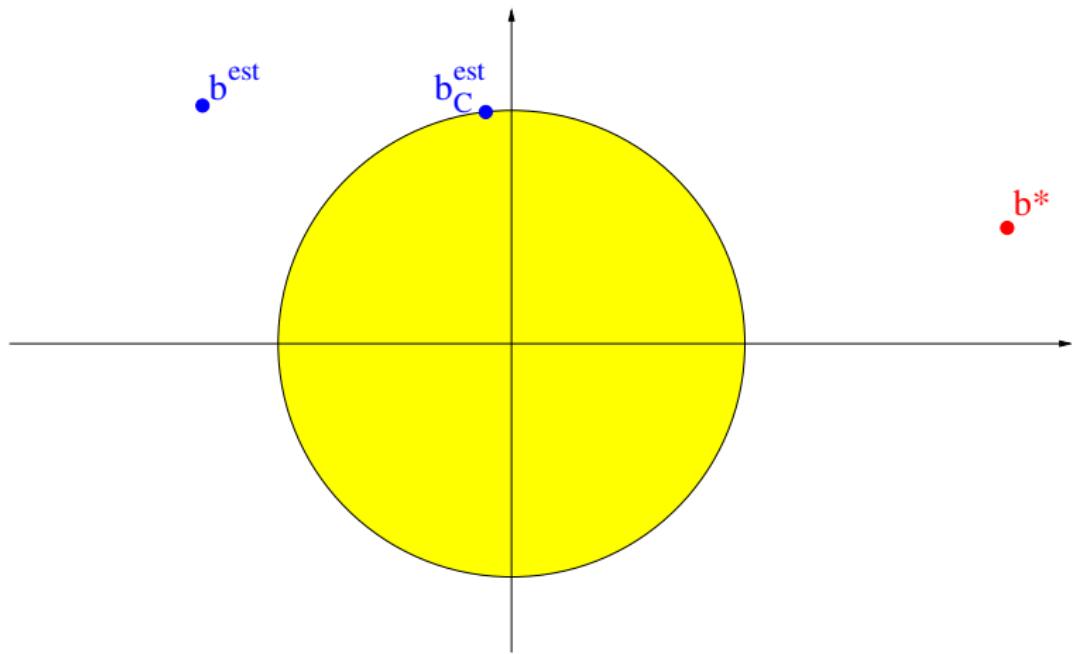
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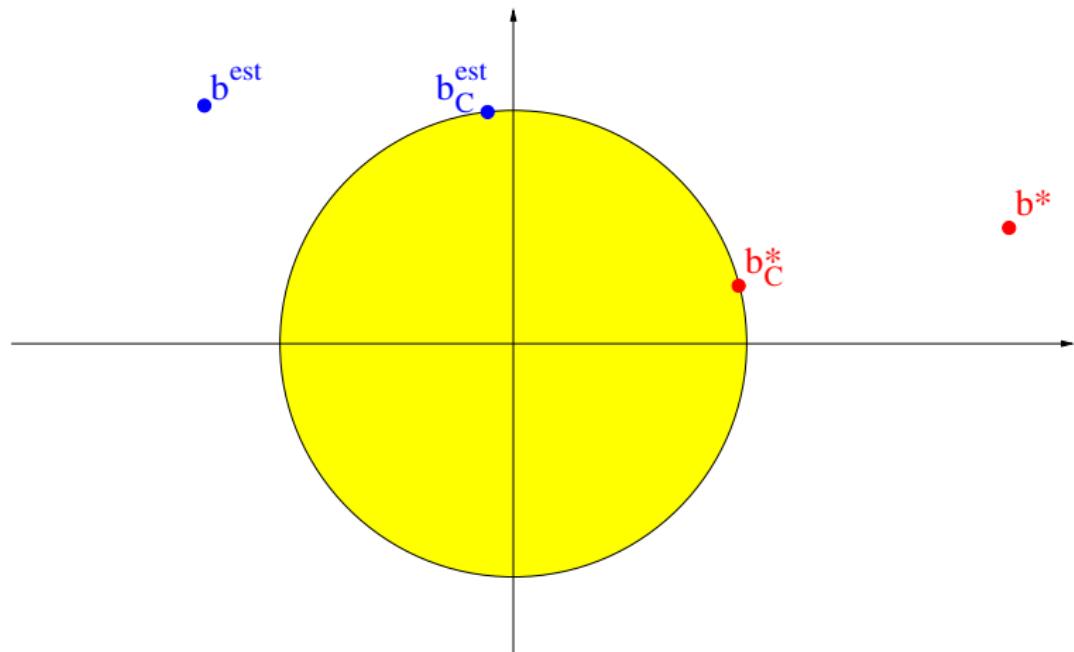
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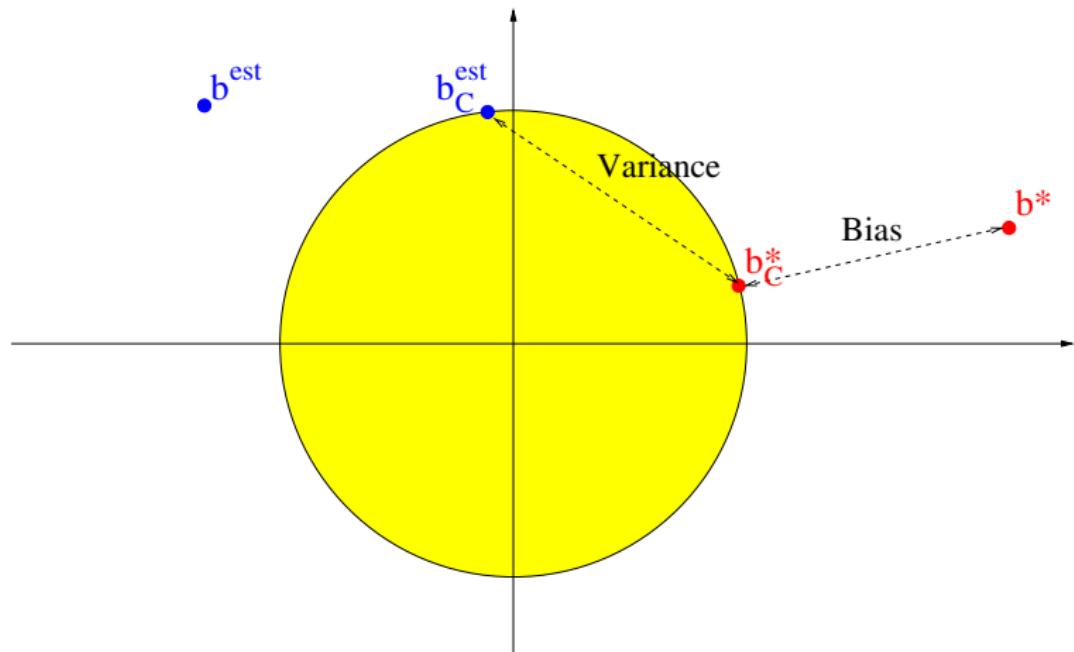
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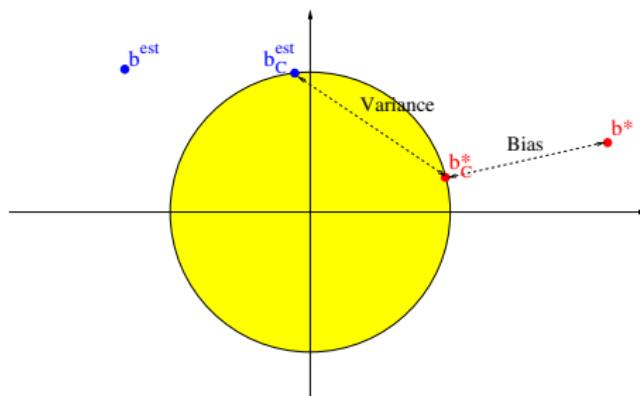
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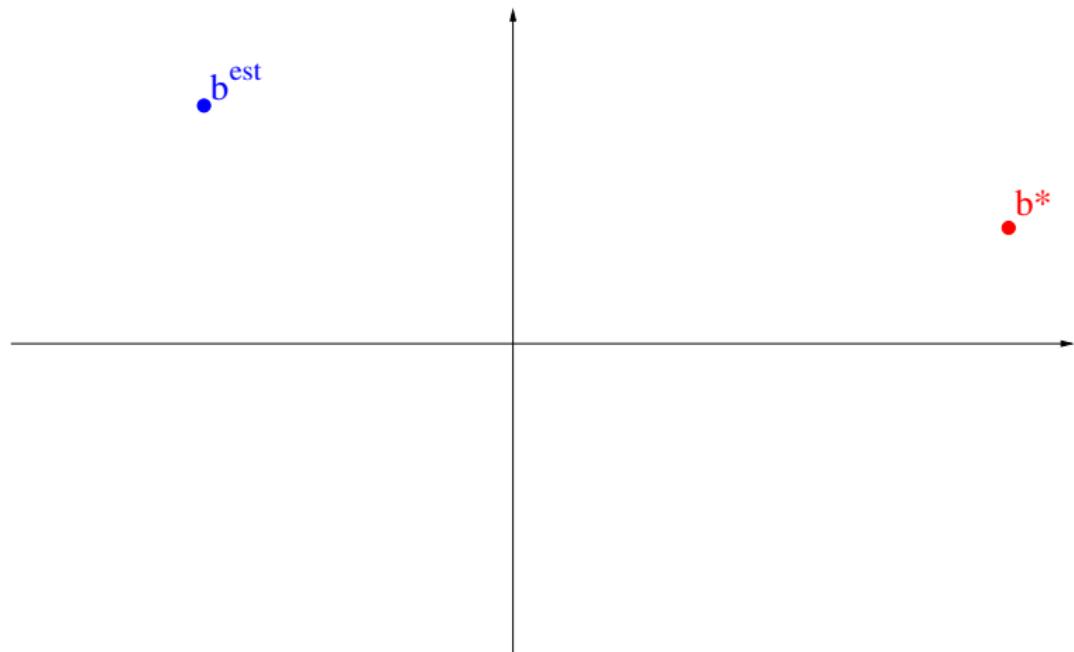
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"Increases bias and decreases variance"

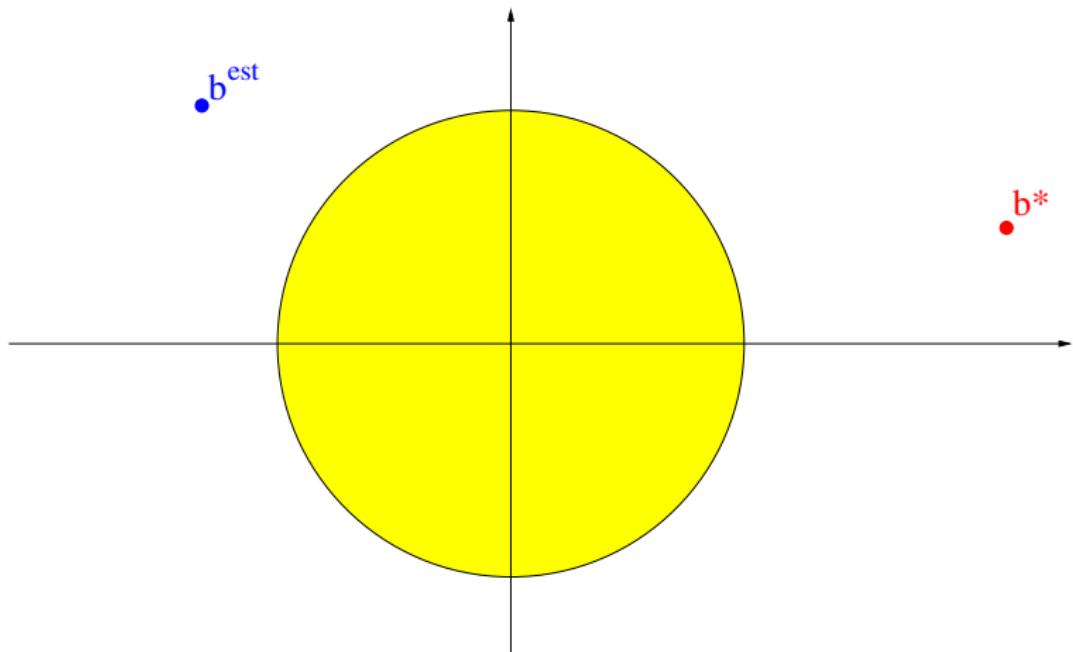
Choice of Ω can decrease the bias

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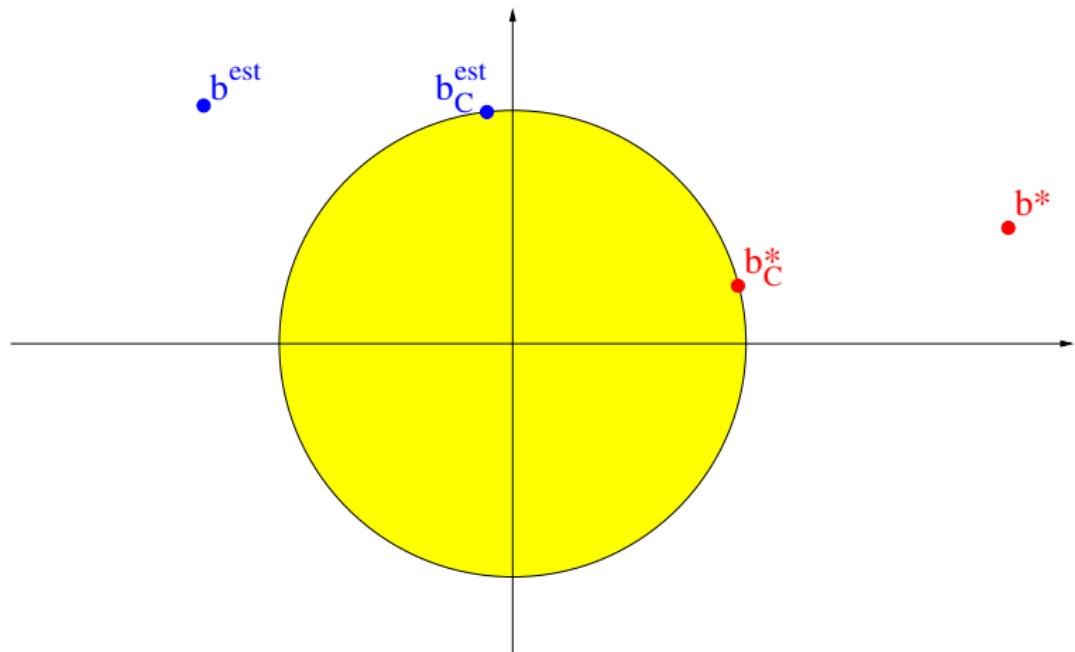
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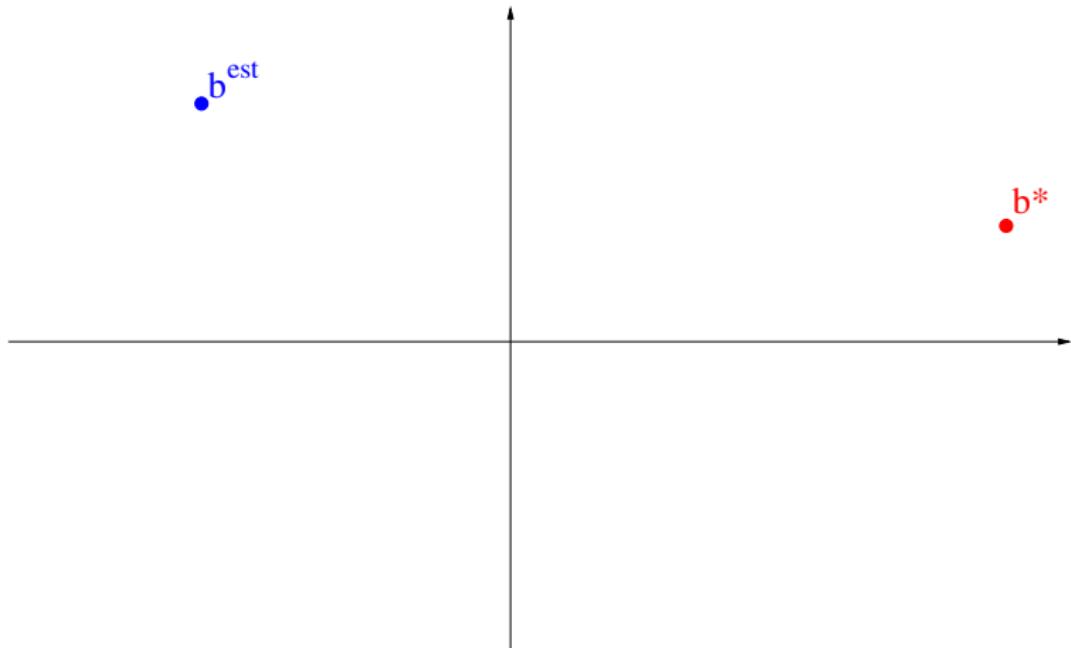
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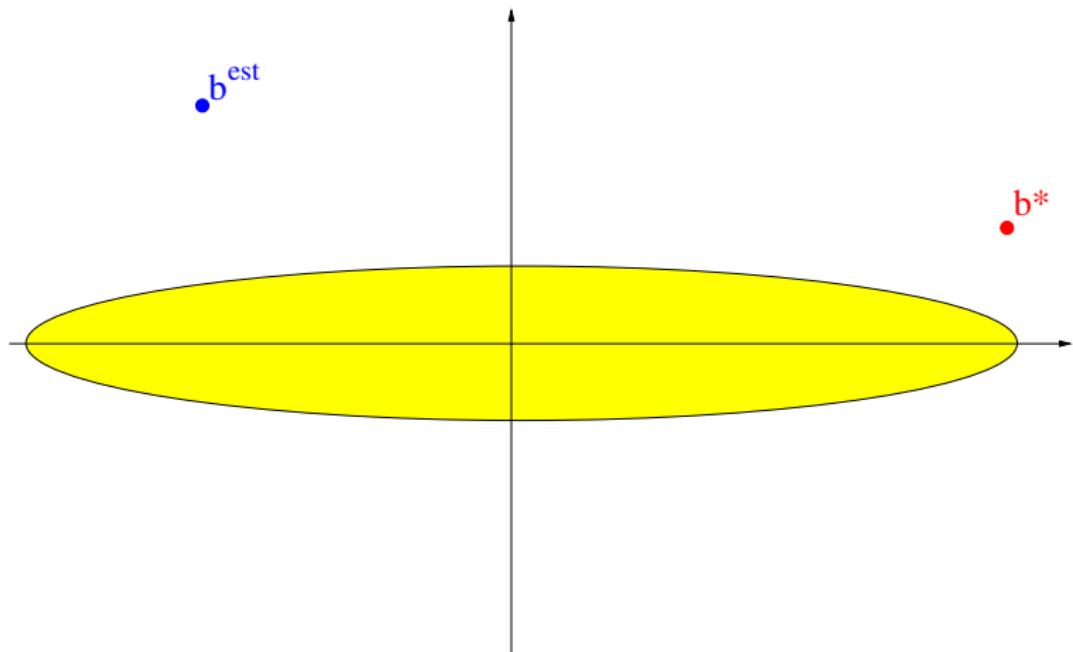
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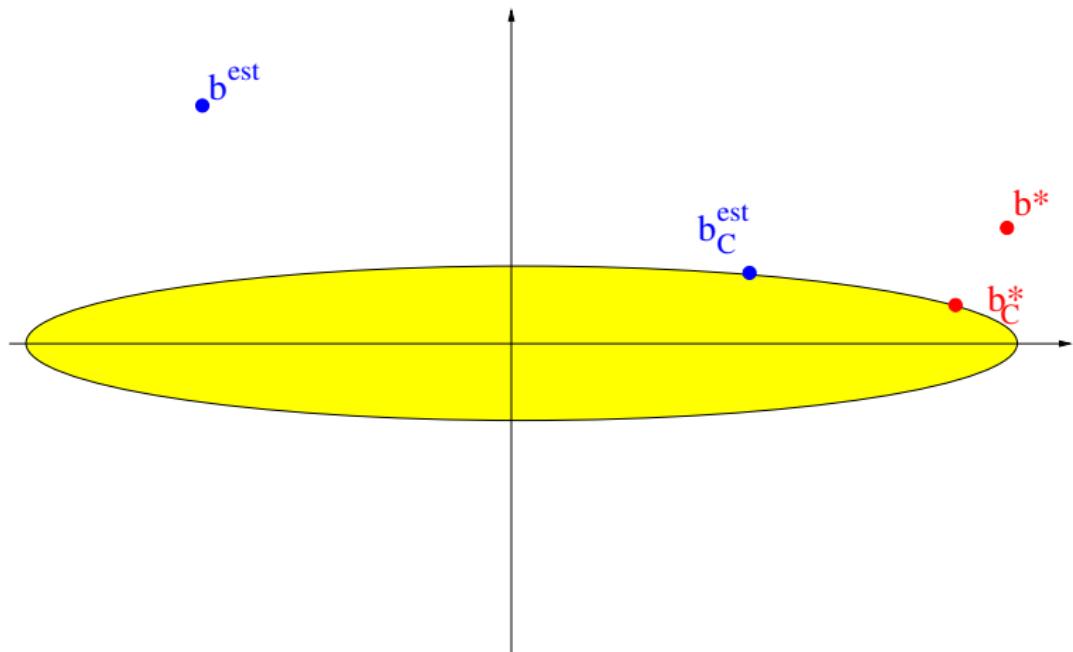
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Equivalent formulation

$$\min_{\beta} R(\beta) \quad \text{subject to} \quad \Omega(\beta) \leq C$$

is equivalent to

$$\min_{\beta} R(\beta) + \lambda \Omega(\beta)$$

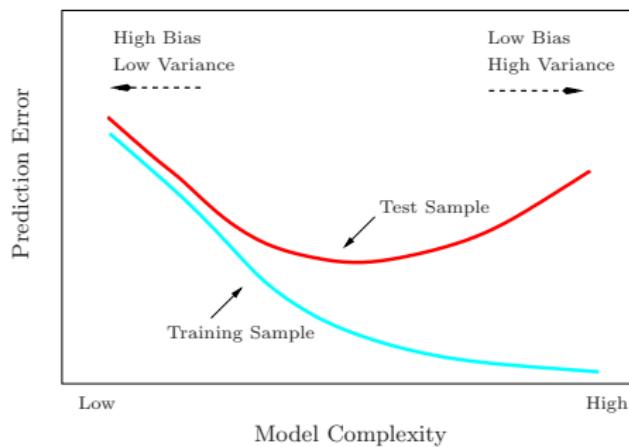
- There exists a (not necessarily unique) correspondance between C and λ such that the solutions to both problems are the same.
- If C increase, λ decreases
- The formulation with λ is often preferred to implement the algorithm
- Proof: using Lagrangian duality (only true under some assumptions, eg, R and Ω convex + Slater conditions, see later)

Choice of C or λ

- Choose a grid of values Λ for λ (or C)
- For each $\lambda \in \Lambda$ (or C) estimate the best model

$$\hat{\beta}_\lambda \in \operatorname{argmin}_\beta R(\beta) + \lambda \Omega(\beta)$$

- Select $\hat{\beta} = \hat{\beta}_{\hat{\lambda}}$ to minimize the bias-variance tradeoff.



Cross-validation

A simple and systematic procedure to estimate the risk (and to optimize the model's parameters)

- ① Randomly divide the training set (of size n) into K (almost) equal portions, each of size K/n
- ② For each portion, fit the model with different parameters on the $K - 1$ other groups and test its performance on the left-out group
- ③ Average performance over the K groups, and take the parameter with the smallest average performance.

Taking $K = 5$ or 10 is recommended as a good default choice.

Summary

- ① Many problems in modern machine learning involve models with many parameters (i.e., high dimension)
- ② The total prediction error of a learning system is the sum of a **bias** and a **variance** error
- ③ In **high dimension**, the **variance** term often dominates
- ④ **Shrinkage methods** allow us to control the bias/variance trade-off
- ⑤ The choice of the **penalty** is where we can put **prior knowledge** to decrease bias
- ⑥ The parameter to control the bias-variance trade-off (C or λ) is typically chosen by **cross-validation**, to minimize the test error.

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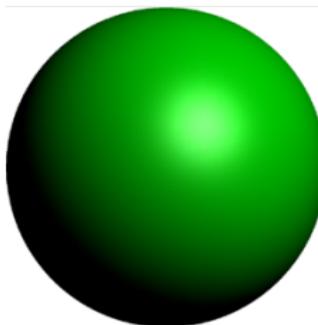
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Overview

- We focus on a simple penalty function: the squared Euclidean norm

$$\Omega(\beta) = \|\beta\|^2 \quad \left(= \beta^\top \beta = \sum_{i=1}^p \beta_i^2 \right)$$



- This will allow us to derive many state-of-the-art linear methods:
 - Ridge regression
 - Ridge logistic regression
 - SVM and large-margin classifiers
- This will allow us to extend these linear methods to nonlinear models, using kernels

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Ridge regression (Hoerl and Kennard, 1970)

- ① Consider the set of linear predictors:

$$\forall \beta \in \mathbb{R}^p, \quad f_\beta(x) = \beta^\top x \quad \text{for } x \in \mathbb{R}^p.$$

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- ② Consider the MSE as empirical risk:

$$R(\beta) = \frac{1}{n} \sum_{i=1}^n (f_\beta(x_i) - y_i)^2.$$

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- ② Consider the MSE as empirical risk:

$$R(\beta) = \frac{1}{n} \sum_{i=1}^n (f_\beta(x_i) - y_i)^2.$$

- ③ Consider the squared Euclidean norm as a penalty:

$$\Omega(\beta) = \|\beta\|^2.$$

Solution

- The penalized risk can be written in matrix form:

$$\begin{aligned} R(\beta) + \lambda \Omega(\beta) &= \frac{1}{n} \sum_{i=1}^n (f_\beta(x_i) - x_i)^2 + \lambda \sum_{i=1}^p \beta_i^2 \\ &= \frac{1}{n} (Y - X\beta)^\top (Y - X\beta) + \lambda \beta^\top \beta. \end{aligned}$$

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- Unique minimizer (by setting the gradient to 0):

$$\hat{\beta}_\lambda^{\text{ridge}} = \arg \min_{\beta \in \mathbb{R}^p} \{R(\beta) + \lambda \Omega(\beta)\} = (X^\top X + \lambda n I)^{-1} X^\top Y.$$

Performance of ridge regression

Lemma

Assume that:

- $Y = X\beta^* + \epsilon$, where $E\epsilon = 0$ and $E\epsilon\epsilon^\top = \sigma^2 I$.
- $X^\top X = nI_p$ (orthogonal design)

Then:

$$\begin{cases} bias(\hat{\beta}_\lambda^{\text{ridge}}) = E(\hat{\beta}_\lambda^{\text{ridge}}) - \beta^* = -\frac{\lambda}{1+\lambda}\beta^*, \\ Var(\hat{\beta}_\lambda^{\text{ridge}}) = \frac{\sigma^2}{n(1+\lambda)^2} I_p = \frac{1}{(1+\lambda)^2} Var(\hat{\beta}^{\text{OLS}}). \end{cases}$$

Proof: exercice

Performance of ridge regression

Corollary

For any $\lambda \geq 0$ let

$$f(\lambda) = E_{S,x_0} \left[\text{bias}^2 \left(x_0^\top \hat{\beta}_\lambda^{\text{ridge}} \right) + \text{Var} \left(x_0^\top \hat{\beta}_\lambda^{\text{ridge}} \right) \right]$$

where $E x_0 = 0$, $E x_0 x_0^\top = I_p$. Then $f(\lambda)$ is minimum for

$$\lambda^* = \frac{\sigma^2 p}{n \|\beta^*\|^2}$$

and

$$f(\lambda^*) = \frac{f(0)f(+\infty)}{f(0) + f(+\infty)} \leq \min \{f(0), f(\infty)\}$$

where

$$f(0) = \sigma^2 p/n, \quad f(\infty) = \|\beta^*\|^2$$

Proof: exercice

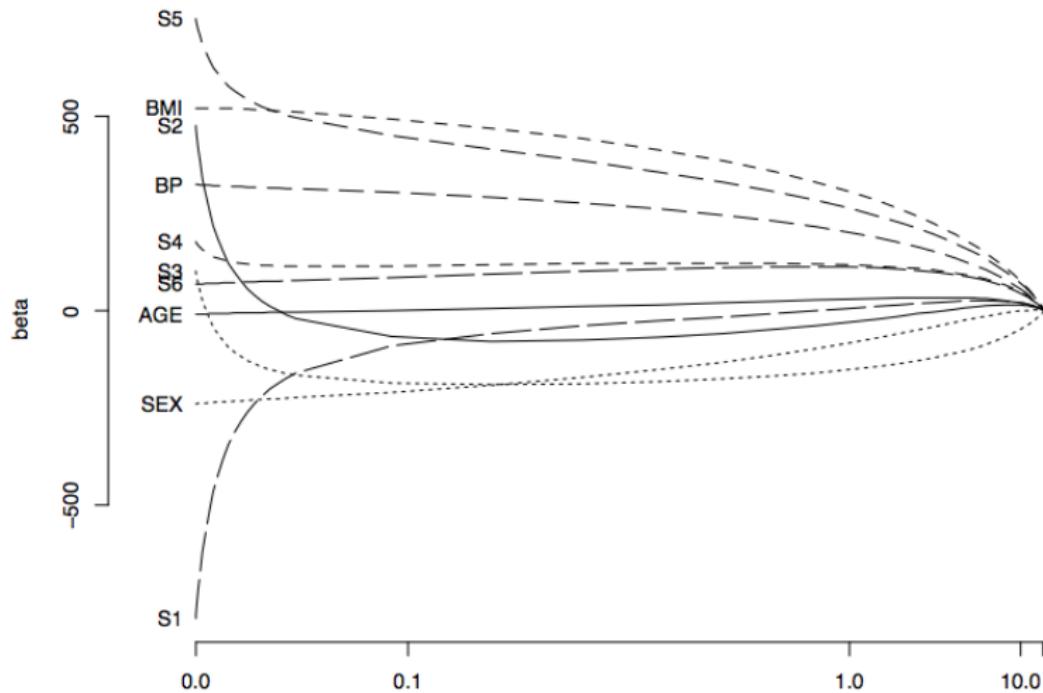
Limit cases

$$\hat{\beta}_\lambda^{\text{ridge}} = (X^\top X + \lambda n I)^{-1} X^\top Y$$

Corollary

- As $\lambda \rightarrow 0$, $\hat{\beta}_\lambda^{\text{ridge}} \rightarrow \hat{\beta}^{\text{OLS}}$ (low bias, high variance).
- As $\lambda \rightarrow +\infty$, $\hat{\beta}_\lambda^{\text{ridge}} \rightarrow 0$ (high bias, low variance).

Ridge regression example



(From Hastie et al., 2001)

Ridge regression with correlated features

Ridge regression is particularly useful in the presence of correlated features:

```
> library(MASS) # for the lm.ridge command
> x1 <- rnorm(20)
> x2 <- rnorm(20,mean=x1,sd=.01)
> y <- rnorm(20,mean=3+x1+x2)
> lm(y~x1+x2)$coef
(Intercept)          x1          x2
 3.070699    25.797872   -23.748019
> lm.ridge(y~x1+x2,lambda=1)
            x1          x2
3.066027 1.015862 0.956560
```

Generalization: ℓ_2 -regularized learning

- A general ℓ_2 -penalized estimator is of the form

$$\min_{\beta} \{ R(\beta) + \lambda \|\beta\|^2 \}, \quad (1)$$

where

$$R(\beta) = \frac{1}{n} \sum_{i=1}^n \ell(f_{\beta}(x_i), y_i)$$

for some general loss functions ℓ .

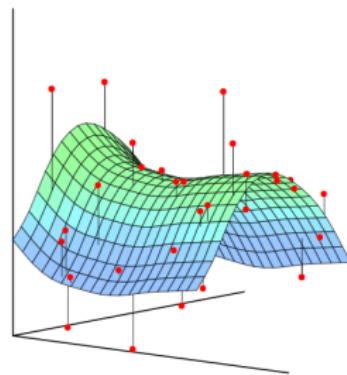
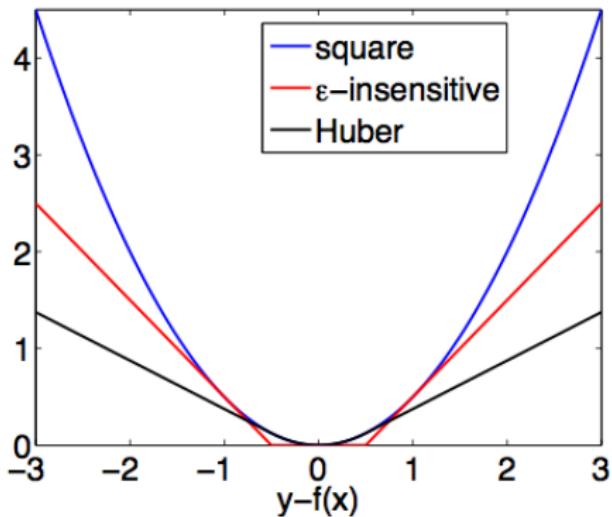
- Ridge regression corresponds to the particular loss

$$\ell(u, y) = (u - y)^2.$$

- For general, **convex** losses, the problem (1) is strictly convex and has a **unique global minimum**, which can usually be found by **numerical algorithms** for convex optimization.

Losses for regression

- Square loss : $\ell(u, y) = (u - y)^2$
- ϵ -insensitive loss : $\ell(u, y) = (|u - y| - \epsilon)_+$
- Huber loss : mixed quadratic/linear



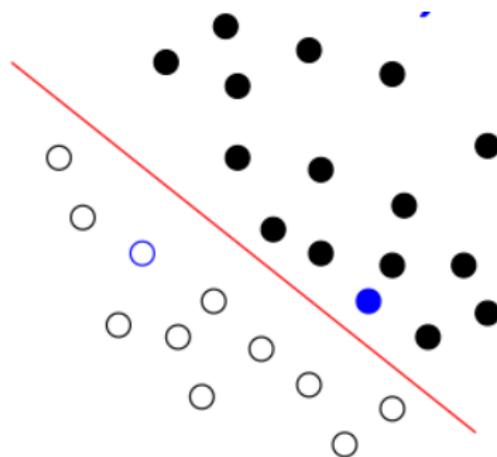
Outline

- 1 Learning in high dimension
- 2 Learning with ℓ_2 regularization
 - Ridge regression
 - Ridge logistic regression
 - Linear hard-margin SVM
 - Interlude: quick notes on constrained optimization
 - Back to hard-margin SVM
 - Soft-margin SVM
 - Large-margin classifiers
- 3 Learning with kernels
 - Kernel methods
 - Positive definite kernels and RKHS
 - Kernel examples
 - Multiple Kernel Learning (MKL)
- 4 Conclusion

Binary classification

Setting

- $\mathcal{X} = \mathbb{R}^p$ set of inputs
- $\mathcal{Y} = \{-1, 1\}$ binary outputs
- $\mathcal{S} = \{(x_1, y_1), \dots, (x_n, y_n)\}$ a training set in $(\mathcal{X} \times \mathcal{Y})^n$
- Goal: Estimate a function $f : \mathcal{X} \rightarrow \mathbb{R}$ to predict y by $\text{sign}(f(x))$



The 0/1 loss

- The 0/1 loss measures if a prediction is correct or not:

$$\ell_{0/1}(f(x), y) = \mathbf{1}(yf(x) < 0) = \begin{cases} 0 & \text{if } y = \text{sign}(f(x)) \\ 1 & \text{otherwise.} \end{cases}$$

- It is then tempting to learn $f_\beta(x) = \beta^\top x$ by solving:

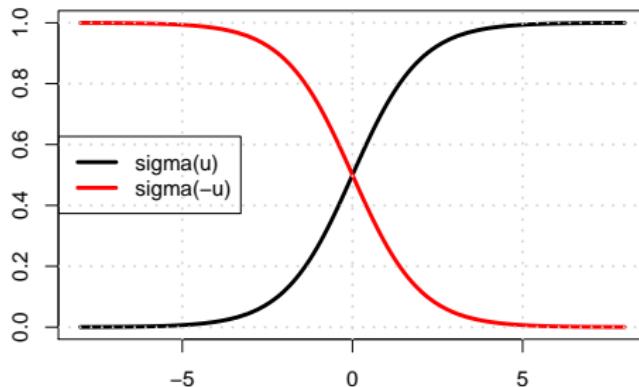
$$\min_{\beta \in \mathbb{R}^p} \underbrace{\frac{1}{n} \sum_{i=1}^n \ell_{0/1}(f_\beta(x_i), y_i)}_{\text{misclassification rate}} + \underbrace{\lambda \|\beta\|^2}_{\text{regularization}}$$

- However:
 - The problem is non-smooth, and typically NP-hard to solve
 - The regularization has **no effect** since the 0/1 loss is invariant by scaling of β
 - In fact, no function achieves the minimum when $\lambda > 0$ (*why?*)

The logistic loss

- An alternative is to define a probabilistic model of y parametrized by $f(x)$, e.g.:

$$\forall y \in \{-1, 1\}, \quad p(y | f(x)) = \frac{1}{1 + e^{-yf(x)}} = \sigma(yf(x))$$



- The **logistic loss** is the negative conditional likelihood:

$$\ell_{logistic}(f(x), y) = -\ln p(y | f(x)) = \ln \left(1 + e^{-yf(x)} \right)$$

Ridge logistic regression (Le Cessie and van Houwelingen, 1992)

$$\min_{\beta \in \mathbb{R}^p} J(\beta) = \frac{1}{n} \sum_{i=1}^n \ln \left(1 + e^{-y_i \beta^\top x_i} \right) + \lambda \|\beta\|^2$$

- Can be interpreted as a regularized conditional maximum likelihood estimator
- No explicit solution, but smooth convex optimization problem that can be solved numerically

Solving ridge logistic regression

$$\min_{\beta} J(\beta) = \frac{1}{n} \sum_{i=1}^n \ln \left(1 + e^{-y_i \beta^\top x_i} \right) + \lambda \|\beta\|^2$$

No explicit solution, but convex problem with:

$$\begin{aligned}\nabla_{\beta} J(\beta) &= -\frac{1}{n} \sum_{i=1}^n \frac{y_i x_i}{1 + e^{y_i \beta^\top x_i}} + 2\lambda\beta \\ &= -\frac{1}{n} \sum_{i=1}^n y_i [1 - P_{\beta}(y_i | x_i)] x_i + 2\lambda\beta\end{aligned}$$

$$\begin{aligned}\nabla_{\beta}^2 J(\beta) &= \frac{1}{n} \sum_{i=1}^n \frac{x_i x_i^\top e^{y_i \beta^\top x_i}}{(1 + e^{y_i \beta^\top x_i})^2} + 2\lambda I \\ &= \frac{1}{n} \sum_{i=1}^n P_{\beta}(1 | x_i) (1 - P_{\beta}(1 | x_i)) x_i x_i^\top + 2\lambda I\end{aligned}$$

Solving ridge logistic regression (cont.)

$$\min_{\beta} J(\beta) = \frac{1}{n} \sum_{i=1}^n \ln \left(1 + e^{-y_i \beta^\top x_i} \right) + \lambda \|\beta\|^2$$

- The solution can then be found by Newton-Raphson iterations:

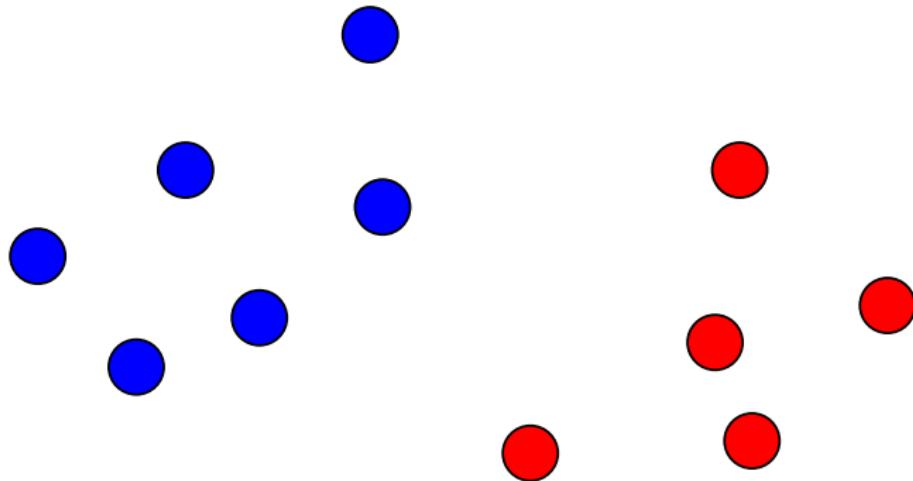
$$\beta^{new} \leftarrow \beta^{old} - \left[\nabla_{\beta}^2 J(\beta^{old}) \right]^{-1} \nabla_{\beta} J(\beta^{old}).$$

- Each step is equivalent to solving a weighted ridge regression problem (*left as exercise*)
- This method is therefore called **iteratively reweighted least squares (IRLS)**.

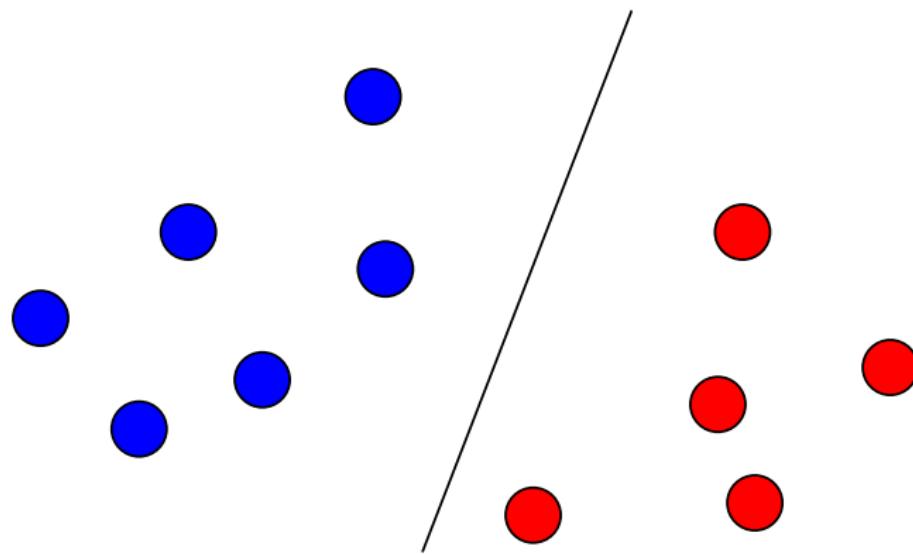
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- 1 Learning in high dimension
- 2 Learning with ℓ_2 regularization
 - Ridge regression
 - Ridge logistic regression
 - Linear hard-margin SVM
 - Interlude: quick notes on constrained optimization
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 - Soft-margin SVM
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- 3 Learning with kernels
 - Kernel methods
 - Positive definite kernels and RKHS
 - Kernel examples
 - Multiple Kernel Learning (MKL)
- 4 Conclusion

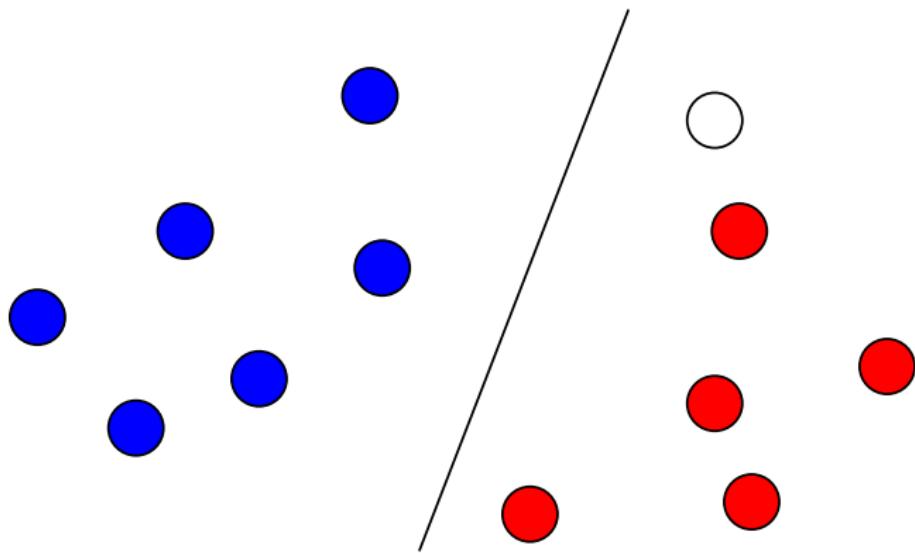
Linear classifier



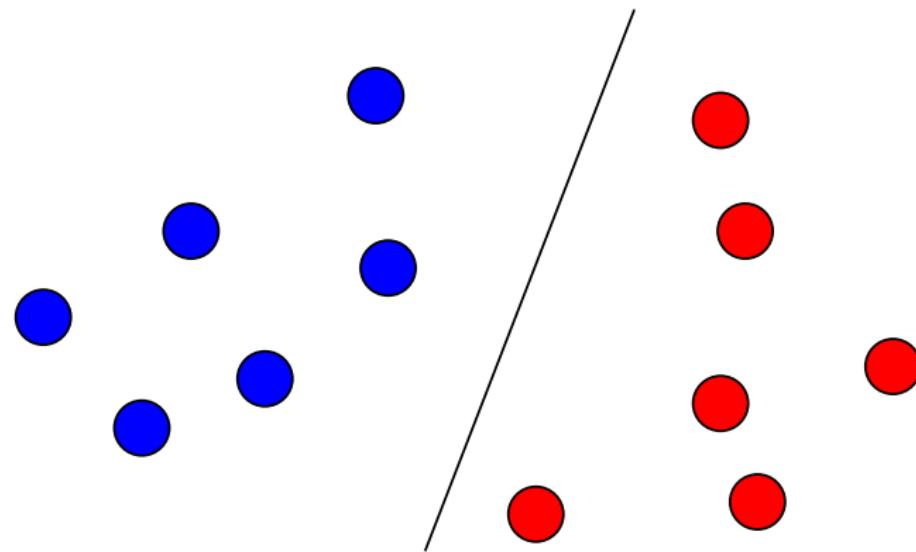
Linear classifier



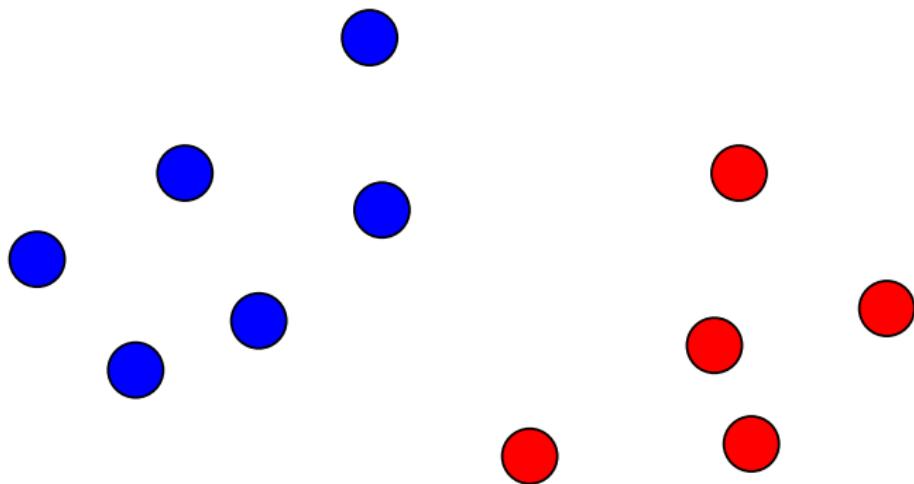
Linear classifier



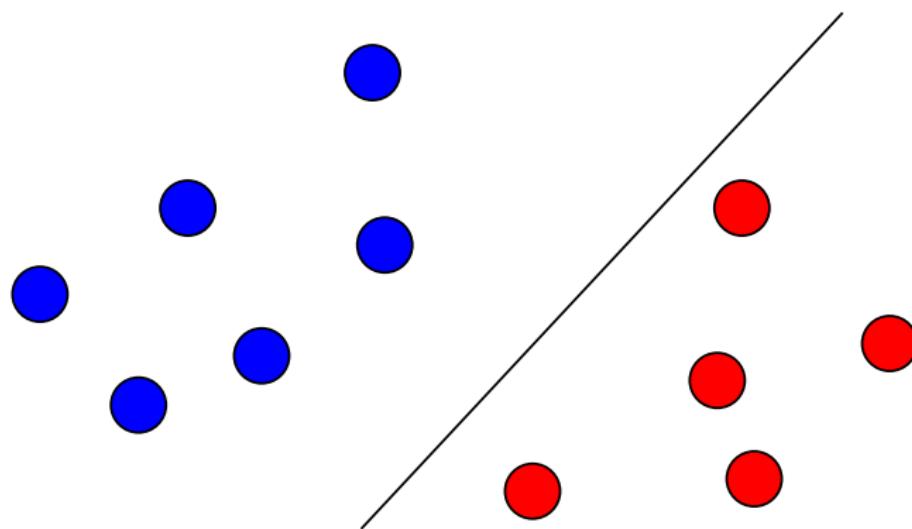
Linear classifier



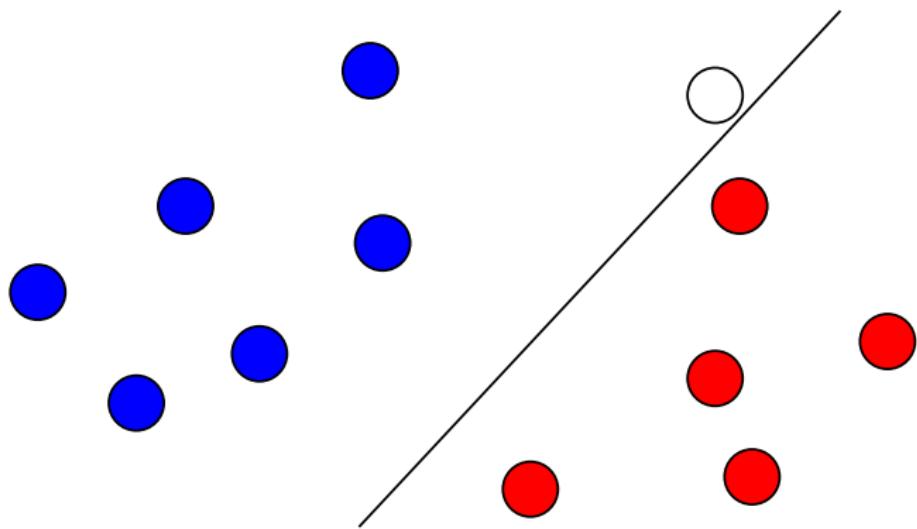
Linear classifier



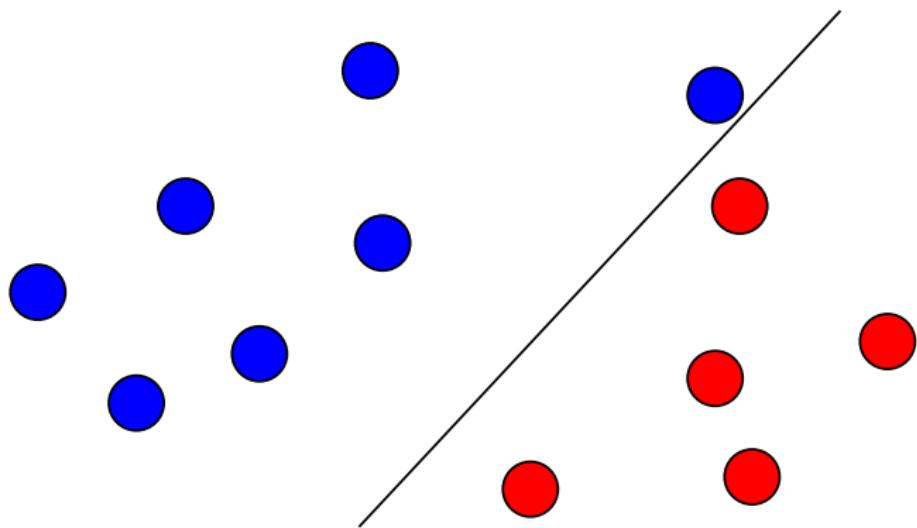
Linear classifier



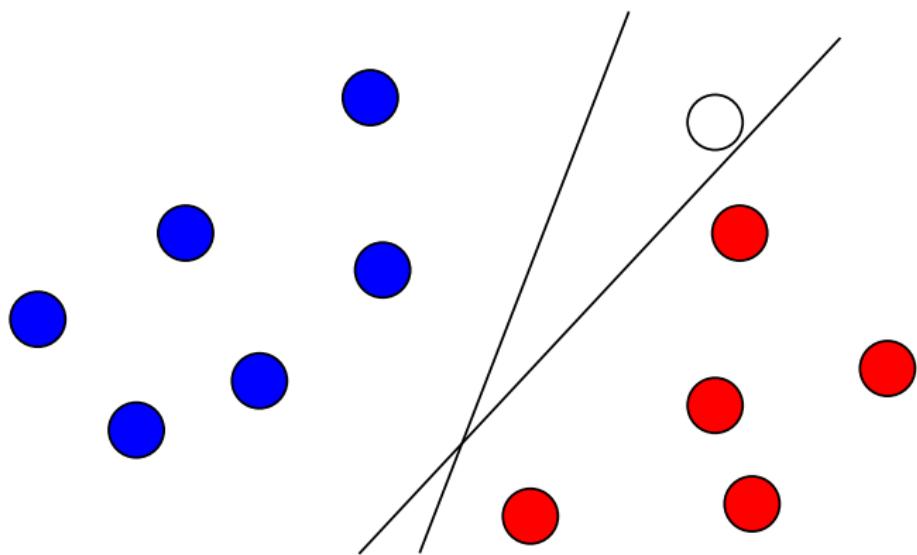
Linear classifier



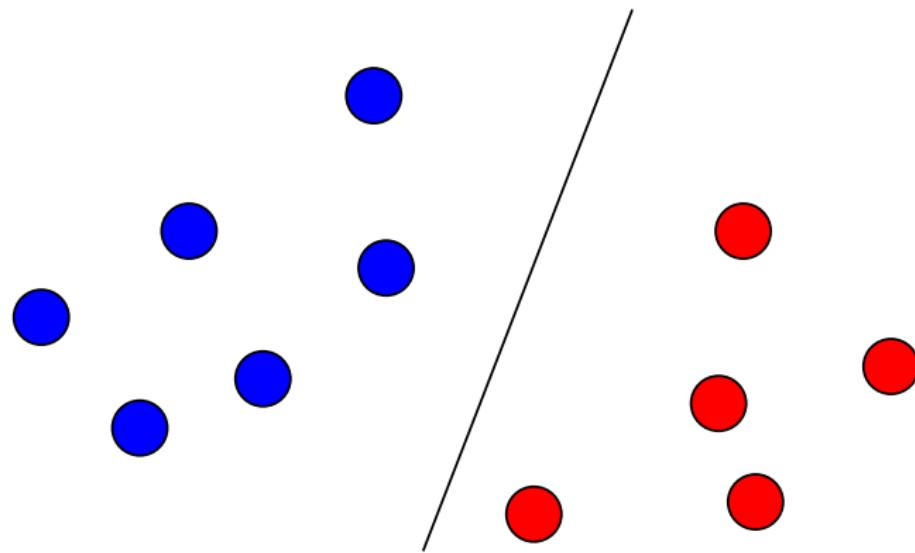
Linear classifier



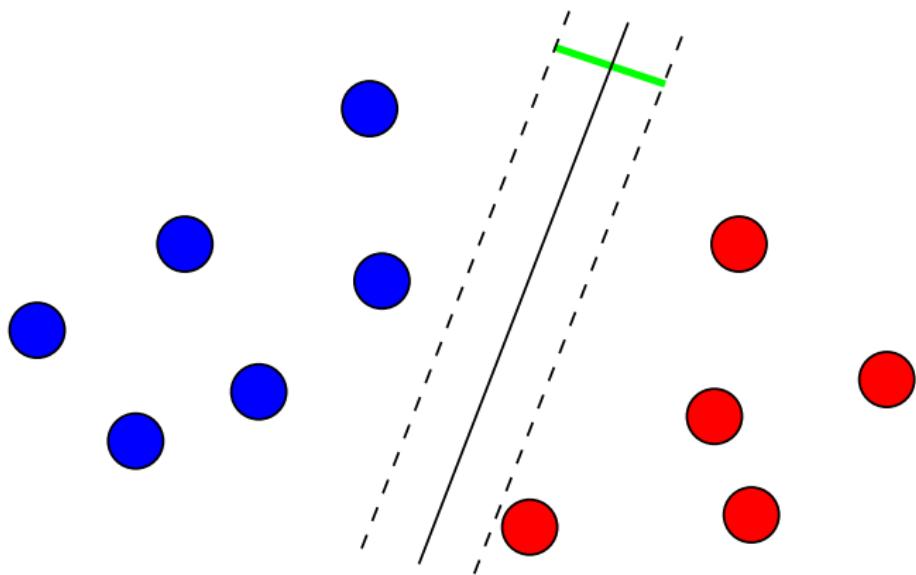
Which one is better?



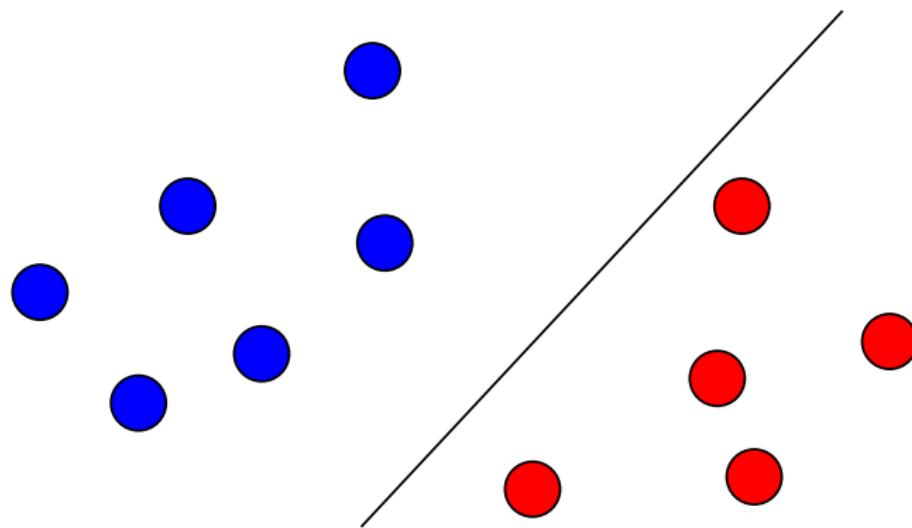
The margin of a linear classifier



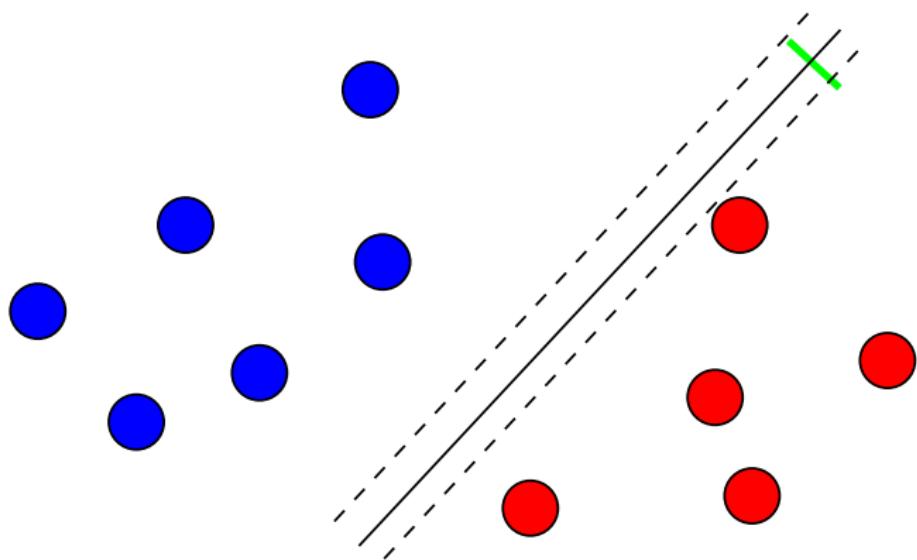
The margin of a linear classifier



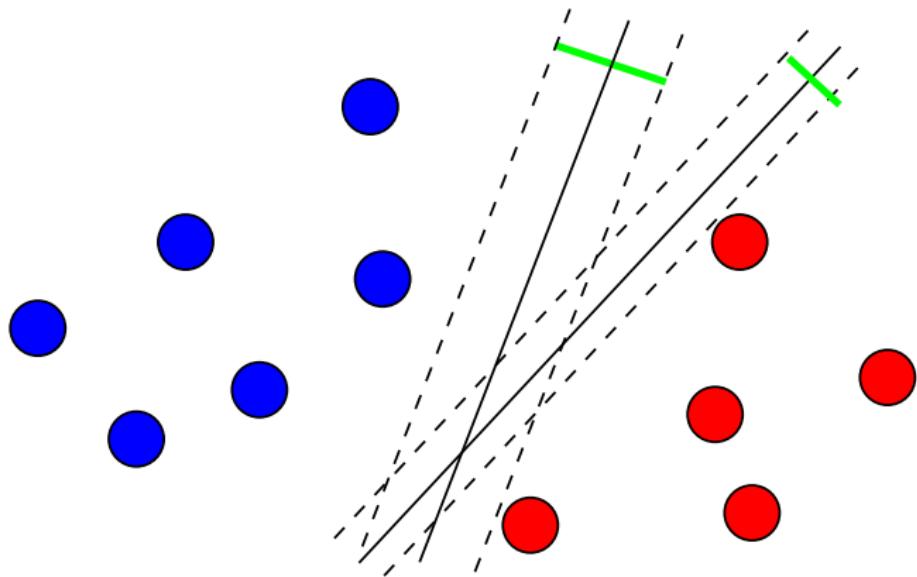
The margin of a linear classifier



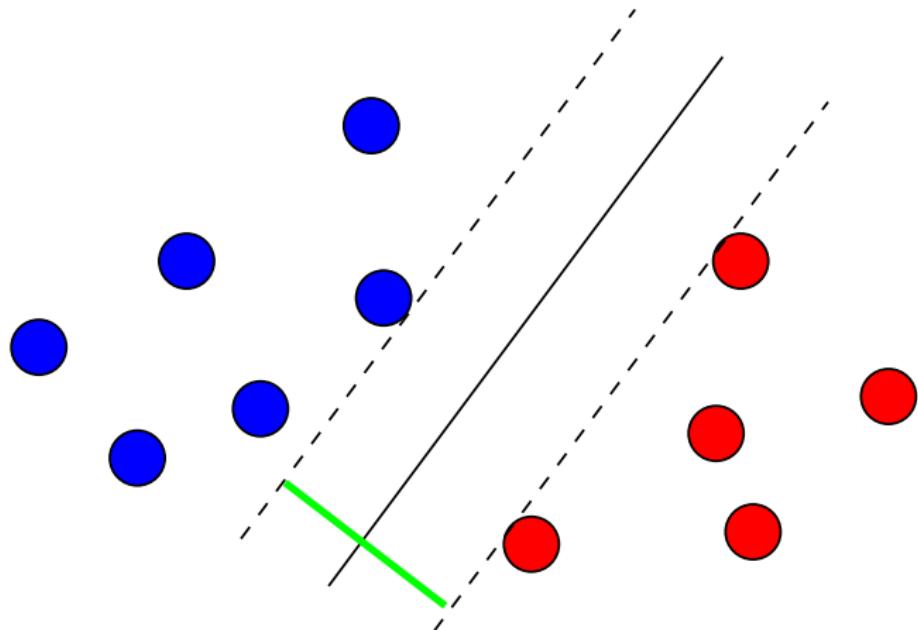
The margin of a linear classifier



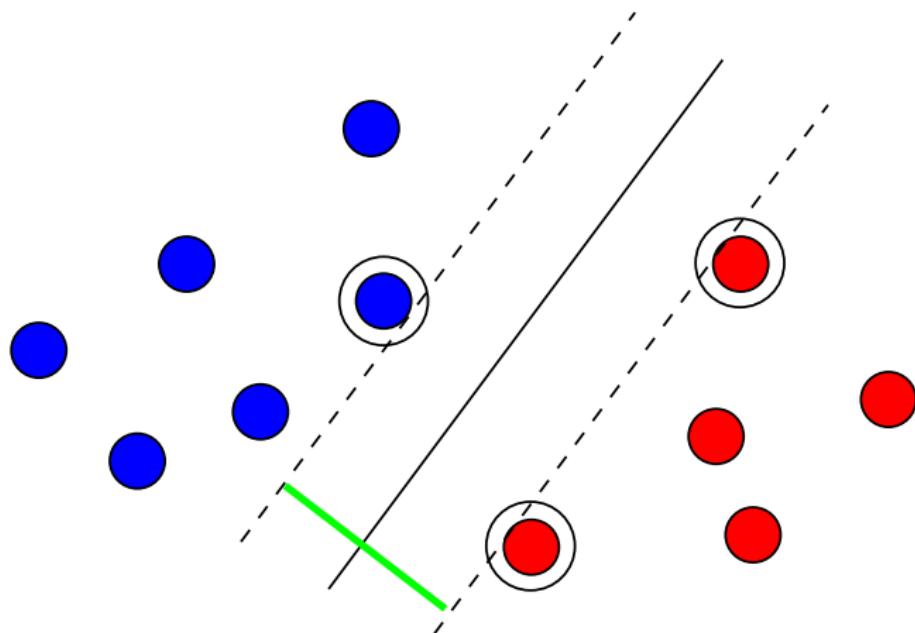
The margin of a linear classifier



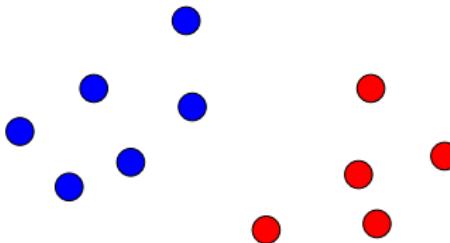
Largest margin classifier (*hard-margin SVM*)



Support vectors



More formally



- The **training set** is a finite set of n data/class pairs:

$$\mathcal{S} = \{(x_1, y_1), \dots, (x_n, y_n)\},$$

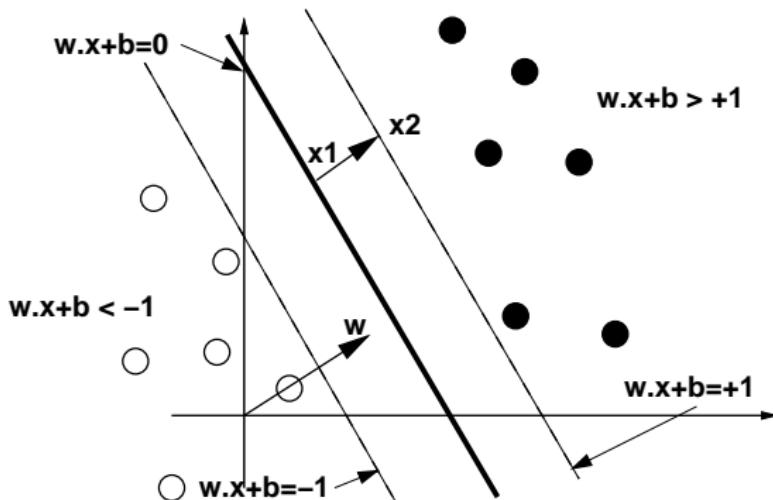
where $x_i \in \mathbb{R}^p$ and $y_i \in \{-1, 1\}$.

- We assume (for the moment) that the data are **linearly separable**, i.e., that there exists $(w, b) \in \mathbb{R}^p \times \mathbb{R}$ such that:

$$\begin{cases} w^\top x_i + b > 0 & \text{if } y_i = 1, \\ w^\top x_i + b < 0 & \text{if } y_i = -1. \end{cases}$$

How to find the largest separating hyperplane?

For a given linear classifier $f(x) = w^\top x + b$ consider the "tube" defined by the values -1 and $+1$ of the decision function:



The margin is $2/\| w \|$

Indeed, the points x_1 and x_2 satisfy:

$$\begin{cases} w^\top x_1 + b = 0, \\ w^\top x_2 + b = 1. \end{cases}$$

By subtracting we get

$$w^\top (x_2 - x_1) = 1 = \| w \| \times \| x_2 - x_1 \|,$$

and therefore:

$$\gamma = 2\| x_2 - x_1 \|_2 = \frac{2}{\| w \|}.$$

All training points should be on the correct side of the dotted line

For positive examples ($y_i = 1$) this means:

$$w^\top x_i + b \geq 1.$$

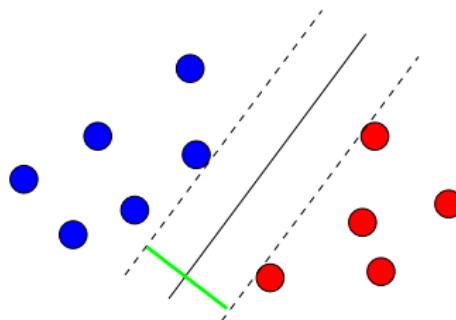
For negative examples ($y_i = -1$) this means:

$$w^\top x_i + b \leq -1.$$

Both cases are summarized by:

$$\forall i = 1, \dots, n, \quad y_i (w^\top x_i + b) \geq 1.$$

Finding the optimal hyperplane



Find (w, b) which minimize:

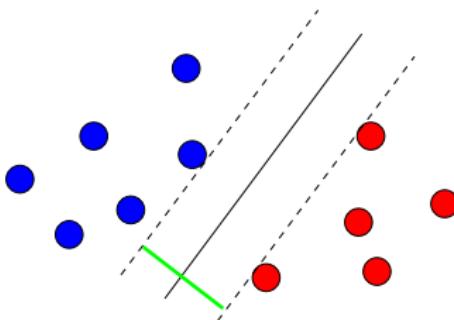
$$\|w\|^2$$

under the constraints:

$$\forall i = 1, \dots, n, \quad y_i (w^\top x_i + b) - 1 \geq 0.$$

This is a classical quadratic program on \mathbb{R}^{p+1} .

Another view of hard-margin SVM



$$\min_{w,b} \left\{ \sum_{i=1}^n \ell_{hard-margin} (w^\top x_i + b, y_i) + \lambda \|w\|^2 \right\},$$

for the hard-margin loss function:

$$\ell_{hard-margin}(u, y) = \begin{cases} 0 & \text{if } yu \geq 1, \\ +\infty & \text{otherwise.} \end{cases}$$

Outline

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- 2 Learning with ℓ_2 regularization
 - Ridge regression
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 - Linear hard-margin SVM
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 - Soft-margin SVM
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 - Kernel methods
 - Positive definite kernels and RKHS
 - Kernel examples
 - Multiple Kernel Learning (MKL)
- 4 Conclusion

Optimization problems

Setting

- We consider an equality and inequality constrained optimization problem over a variable $x \in \mathcal{X}$:

$$\text{minimize } f(x)$$

$$\text{subject to } h_i(x) = 0, \quad i = 1, \dots, m,$$

$$g_j(x) \leq 0, \quad j = 1, \dots, r,$$

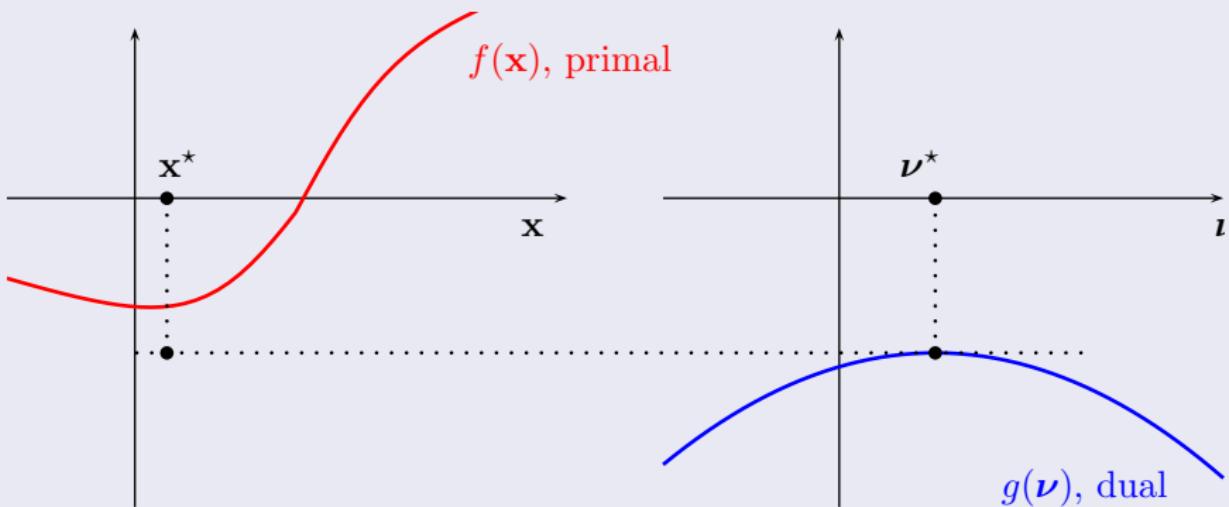
making **no assumption** of f , g and h .

- Let us denote by f^* the optimal value of the decision function under the constraints, i.e., $f^* = f(x^*)$ if the minimum is reached at a global minimum x^* .

Duality

Duality provides of a concave *dual* function q from a *primal* function f such that for all pair x, ν , the value $f(x)$ is greater than $q(\nu)$.

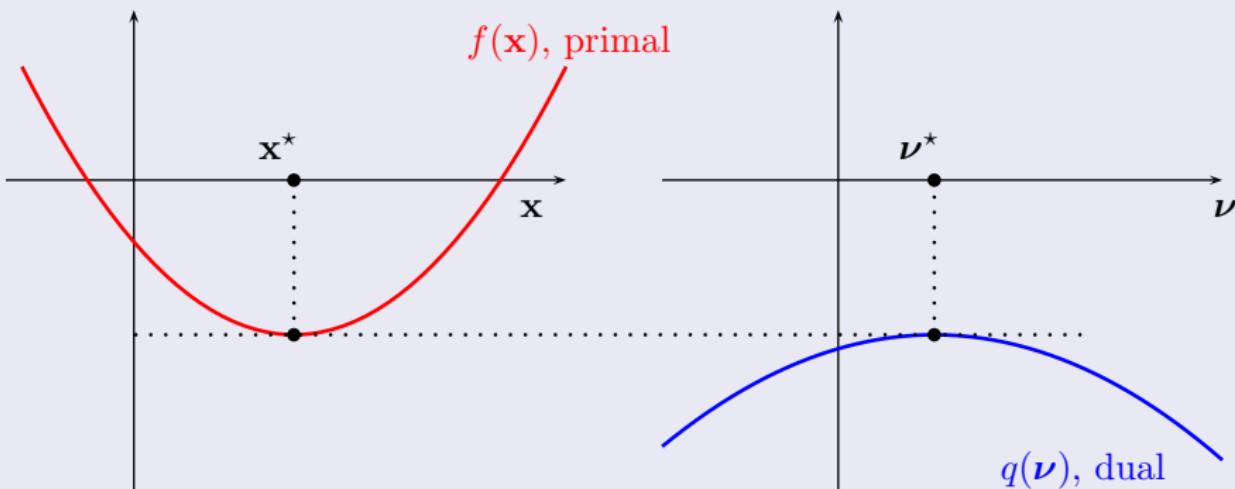
Weak Duality



Duality

For most “reasonable” convex problems, duality comes with an additional property called strong duality, which is very useful.

Strong Duality

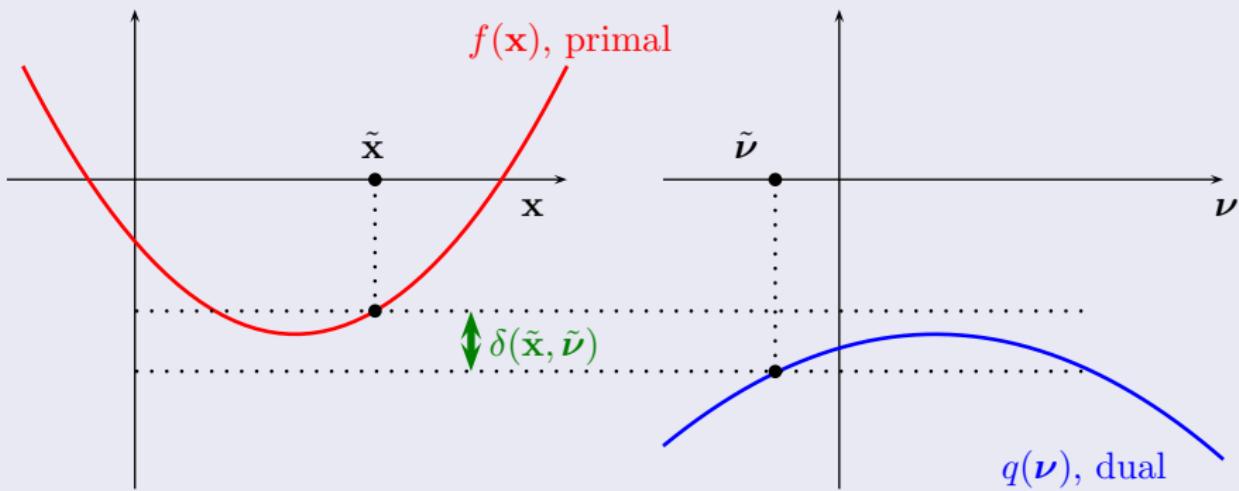


- Strong duality means that $\max_{\nu} q(\nu) = \min_{\mathbf{x}} f(\mathbf{x})$

Duality

For instance, we have the concept of duality gap, which are very useful to stop an optimization algorithm.

Duality gaps



- The duality gap guarantees us that $0 \leq f(\tilde{\mathbf{x}}) - f(\mathbf{x}^*) \leq \delta(\tilde{\mathbf{x}}, \tilde{\nu})$.
- Dual problems are often obtained by Lagrangian or Fenchel duality.

Optimization problems

Setting

- We consider an equality and inequality constrained optimization problem over a variable $x \in \mathcal{X}$:

$$\text{minimize } f(x)$$

$$\text{subject to } h_i(x) = 0, \quad i = 1, \dots, m,$$

$$g_j(x) \leq 0, \quad j = 1, \dots, r,$$

making **no assumption** of f , g and h .

- Let us denote by f^* the optimal value of the decision function under the constraints, i.e., $f^* = f(x^*)$ if the minimum is reached at a global minimum x^* .

Lagrangian and dual function

Lagrangian

The **Lagrangian** of this problem is the function $L : \mathcal{X} \times \mathbb{R}^m \times \mathbb{R}^r \rightarrow \mathbb{R}$ defined by:

$$L(x, \lambda, \mu) = f(x) + \sum_{i=1}^m \lambda_i h_i(x) + \sum_{j=1}^r \mu_j g_j(x).$$

Lagrangian dual function

The **Lagrange dual function** $g : \mathbb{R}^m \times \mathbb{R}^r \rightarrow \mathbb{R}$ is:

$$\begin{aligned} q(\lambda, \mu) &= \inf_{x \in \mathcal{X}} L(x, \lambda, \mu) \\ &= \inf_{x \in \mathcal{X}} \left(f(x) + \sum_{i=1}^m \lambda_i h_i(x) + \sum_{j=1}^r \mu_j g_j(x) \right). \end{aligned}$$

Properties of the dual function

- q is concave in (λ, μ) , even if the original problem is not convex.
- The dual function yields lower bounds on the optimal value f^* of the original problem when μ is nonnegative:

$$q(\lambda, \mu) \leq f^* , \quad \forall \lambda \in \mathbb{R}^m, \forall \mu \in \mathbb{R}^r, \mu \geq 0 .$$

Proofs

- For each x , the function $(\lambda, \mu) \mapsto L(x, \lambda, \mu)$ is linear, and therefore both convex and concave in (λ, μ) . The pointwise minimum of concave functions is concave, therefore q is concave.
- Let \bar{x} be any feasible point, i.e., $h(\bar{x}) = 0$ and $g(\bar{x}) \leq 0$. Then we have, for any λ and $\mu \geq 0$:

$$\sum_{i=1}^m \lambda_i h_i(\bar{x}) + \sum_{i=1}^r \mu_i g_i(\bar{x}) \leq 0 ,$$

$$\implies L(\bar{x}, \lambda, \mu) = f(\bar{x}) + \sum_{i=1}^m \lambda_i h_i(\bar{x}) + \sum_{i=1}^r \mu_i g_i(\bar{x}) \leq f(\bar{x}) ,$$

$$\implies q(\lambda, \mu) = \inf_x L(x, \lambda, \mu) \leq L(\bar{x}, \lambda, \mu) \leq f(\bar{x}) , \quad \forall \bar{x} . \quad \square$$

Dual problem

Definition

For the (primal) problem:

$$\begin{aligned} & \text{minimize} && f(x) \\ & \text{subject to} && h(x) = 0 , \quad g(x) \leq 0 , \end{aligned}$$

the Lagrange dual problem is:

$$\begin{aligned} & \text{maximize} && q(\lambda, \mu) \\ & \text{subject to} && \mu \geq 0 , \end{aligned}$$

where q is the (concave) Lagrange dual function and λ and μ are the Lagrange multipliers associated to the constraints $h(x) = 0$ and $g(x) \leq 0$.

Weak duality

- Let d^* the optimal value of the Lagrange dual problem. Each $q(\lambda, \mu)$ is an lower bound for f^* and by definition d^* is the best lower bound that is obtained. The following **weak duality inequality** therefore always hold:

$$d^* \leq f^* .$$

- This inequality holds when d^* or f^* are infinite. The difference $d^* - f^*$ is called the **optimal duality gap** of the original problem.

Strong duality

- We say that **strong duality** holds if the optimal duality gap is zero, i.e.:

$$d^* = f^* .$$

- If strong duality holds, then the best lower bound that can be obtained from the Lagrange dual function is **tight**
- Strong duality does **not hold** for general nonlinear problems.
- It usually holds for **convex problems**.
- Conditions that ensure strong duality for convex problems are called **constraint qualification**.

Slater's constraint qualification

Strong duality holds for a **convex** problem:

$$\begin{aligned} & \text{minimize} && f(x) \\ & \text{subject to} && g_j(x) \leq 0, \quad j = 1, \dots, r, \\ & && Ax = b, \end{aligned}$$

if it is **strictly feasible**, i.e., there exists at least one **feasible point** that satisfies:

$$g_j(x) < 0, \quad j = 1, \dots, r, \quad Ax = b.$$

Remarks

- Slater's conditions also ensure that the maximum d^* (if $> -\infty$) is attained, i.e., there exists a point (λ^*, μ^*) with

$$q(\lambda^*, \mu^*) = d^* = f^*$$

- They can be sharpened. For example, strict feasibility is not required for affine constraints.
- There exist many other types of constraint qualifications

Dual optimal pairs

Suppose that strong duality holds, x^* is primal optimal, (λ^*, μ^*) is dual optimal. Then we have:

$$\begin{aligned} f(x^*) &= q(\lambda^*, \mu^*) \\ &= \inf_{x \in \mathbb{R}^n} \left\{ f(x) + \sum_{i=1}^m \lambda_i^* h_i(x) + \sum_{j=1}^r \mu_j^* g_j(x) \right\} \\ &\leq f(x^*) + \sum_{i=1}^m \lambda_i^* h_i(x^*) + \sum_{j=1}^r \mu_j^* g_j(x^*) \\ &\leq f(x^*) \end{aligned}$$

Hence both inequalities are in fact **equalities**.

Complimentary slackness

The first equality shows that:

$$L(x^*, \lambda^*, \mu^*) = \inf_{x \in \mathbb{R}^n} L(x, \lambda^*, \mu^*) ,$$

showing that x^* minimizes the Lagrangian at (λ^*, μ^*) . The second equality shows that:

$$\mu_j g_j(x^*) = 0 , \quad j = 1, \dots, r .$$

This property is called complementary slackness:
the i th optimal Lagrange multiplier is zero unless the i th constraint is active at the optimum.

Outline

- 1 Learning in high dimension
- 2 Learning with ℓ_2 regularization
 - Ridge regression
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 - Interlude: quick notes on constrained optimization
 - Back to hard-margin SVM
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- 3 Learning with kernels
 - Kernel methods
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 - Kernel examples
 - Multiple Kernel Learning (MKL)
- 4 Conclusion

Lagrangian

In order to minimize:

$$\frac{1}{2} \|w\|^2$$

under the constraints:

$$\forall i = 1, \dots, n, \quad y_i (w^\top x_i + b) - 1 \geq 0,$$

we introduce one dual variable α_i for each constraint, i.e., for each training point. The Lagrangian is:

$$L(w, b, \alpha) = \frac{1}{2} \|w\|^2 - \sum_{i=1}^n \alpha_i (y_i (w^\top x_i + b) - 1).$$

Lagrangian

- $L(w, b, \alpha)$ is convex quadratic in w . It is minimize for:

$$\nabla_w L = w - \sum_{i=1}^n \alpha_i y_i x_i = 0 \quad \Rightarrow \quad w = \sum_{i=1}^n \alpha_i y_i x_i.$$

- $L(w, b, \alpha)$ is affine in b . Its minimum is $-\infty$ except if:

$$\nabla_b L = \sum_{i=1}^n \alpha_i y_i = 0.$$

Dual function

- We therefore obtain the **Lagrange dual function**:

$$q(\alpha) = \inf_{w \in \mathbb{R}^p, b \in \mathbb{R}} L(w, b, \alpha)$$
$$= \begin{cases} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n y_i y_j \alpha_i \alpha_j x_i \cdot x_j & \text{if } \sum_{i=1}^n \alpha_i y_i = 0, \\ -\infty & \text{otherwise.} \end{cases}$$

- The dual problem is:

$$\begin{aligned} & \text{maximize } q(\alpha) \\ & \text{subject to } \alpha \geq 0. \end{aligned}$$

Dual problem

Find $\alpha^* \in \mathbb{R}^n$ which maximizes

$$L(\alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j x_i^\top x_j,$$

under the (simple) constraints $\alpha_i \geq 0$ (for $i = 1, \dots, n$), and

$$\sum_{i=1}^n \alpha_i y_i = 0.$$

This is a quadratic program on \mathbb{R}^N , with "box constraints". α^ can be found efficiently using dedicated optimization softwares.*

Complementary slackness conditions

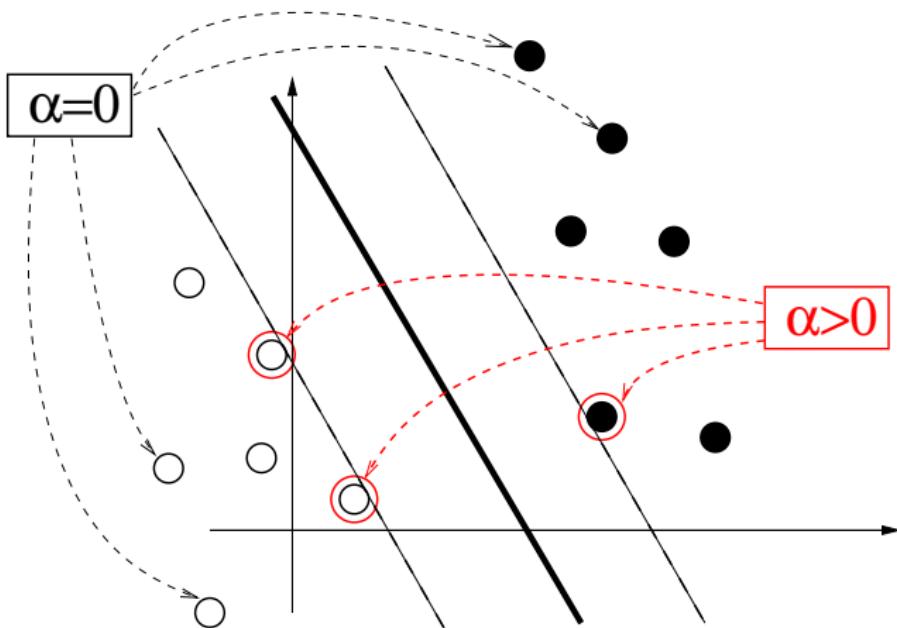
- At the optimal, the complementary slackness conditions must hold:

$$\forall i = 1, \dots, n \quad \alpha_i^* \left(y_i \left(w^{*\top} x_i + b^* \right) - 1 \right) = 0.$$

- This implies that:

- If $\alpha_i^* > 0$ then $y_i \left(w^{*\top} x_i + b^* \right) = 1$
- If $y_i \left(w^{*\top} x_i + b^* \right) > 1$ then $\alpha_i^* = 0$

Interpretation: support vectors



Recovering the optimal hyperplane

- Once α^* is found, we recover w^* by:

$$w^* = \underset{w}{\operatorname{argmin}} L(w, b, \alpha^*) = \sum_{i=1}^n \alpha_i y_i x_i$$

- To recover b we can not just minimize $L(w, b, \alpha^*)$, since it does not depend on b . Instead, we use the complementary slackness condition: if i is such that $\alpha_i > 0$, then

$$y_i (w^{*\top} x_i + b^*) = 1 \implies b^* = y_i - w^{*\top} x_i$$

- The **decision function** is therefore:

$$\begin{aligned} f^*(x) &= w^{*\top} x + b^* \\ &= \sum_{i=1}^n \alpha_i y_i x_i^\top x + b^*. \end{aligned}$$

Primal (for large n) vs dual (for large p) optimization

- ① Find $(w, b) \in \mathbb{R}^{p+1}$ which minimize:

$$\frac{1}{2} \| w \|^2$$

under the constraints:

$$\forall i = 1, \dots, n, \quad y_i (w^\top x_i + b) - 1 \geq 0.$$

- ② Find $\alpha^* \in \mathbb{R}^n$ which maximizes

$$L(\alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j x_i \cdot x_j,$$

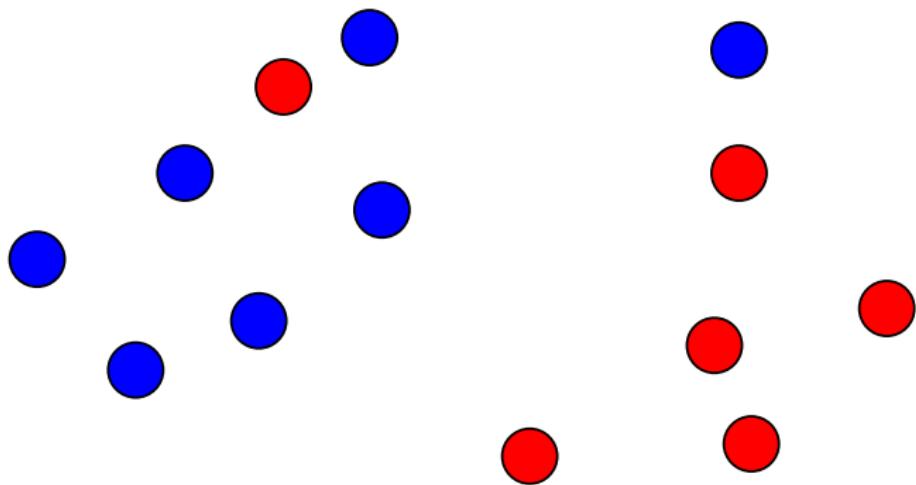
under the (simple) constraints $\alpha_i \geq 0$ (for $i = 1, \dots, n$), and

$$\sum_{i=1}^n \alpha_i y_i = 0.$$

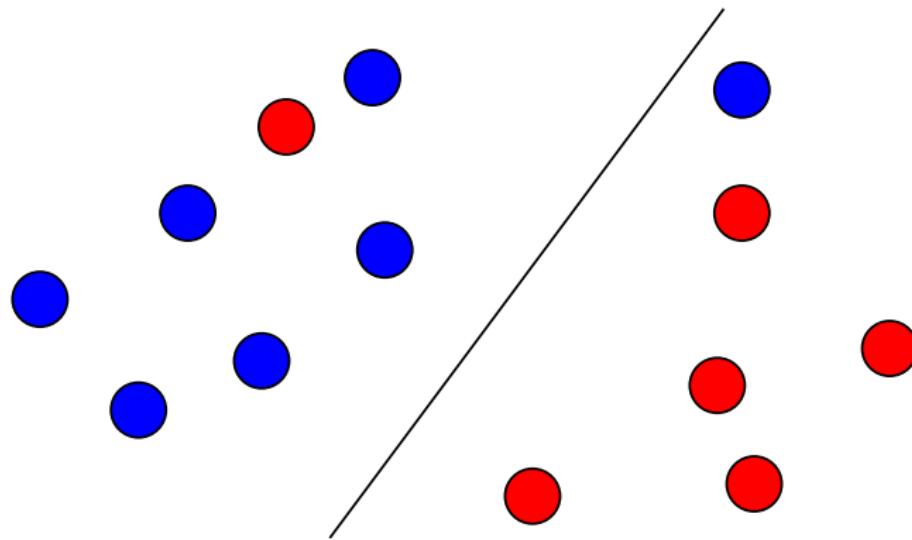
Outline

- 1 Learning in high dimension
- 2 Learning with ℓ_2 regularization
 - Ridge regression
 - Ridge logistic regression
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 - Interlude: quick notes on constrained optimization
 - Back to hard-margin SVM
 - Soft-margin SVM
 - Large-margin classifiers
- 3 Learning with kernels
 - Kernel methods
 - Positive definite kernels and RKHS
 - Kernel examples
 - Multiple Kernel Learning (MKL)
- 4 Conclusion

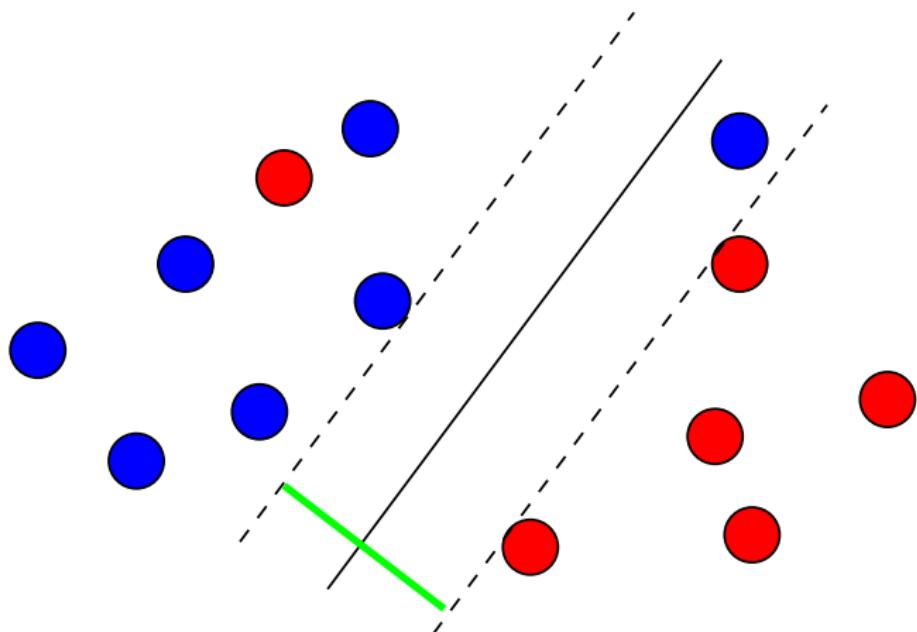
What if data are not linearly separable?



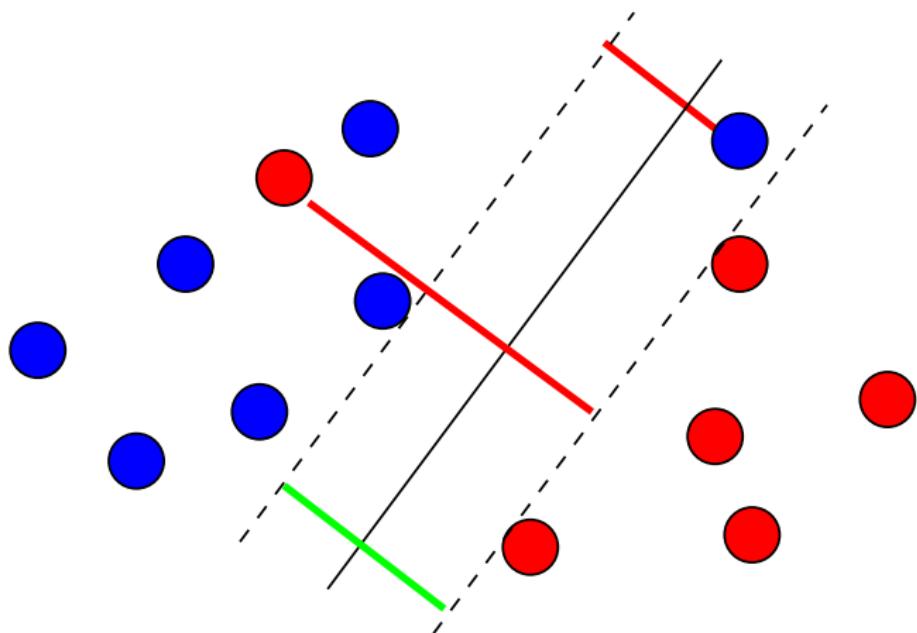
What if data are not linearly separable?



What if data are not linearly separable?



What if data are not linearly separable?

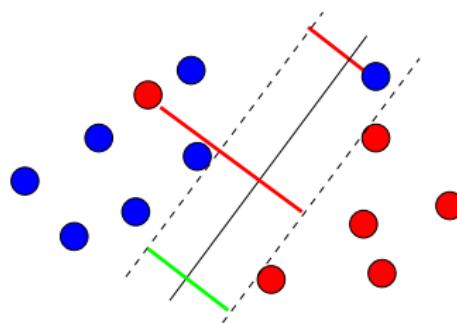


Soft-margin SVM

- Find a trade-off between **large margin** and **few errors**.
- Mathematically:

$$\min_f \left\{ \frac{1}{margin(f)} + C \times errors(f) \right\}$$

- C is a parameter



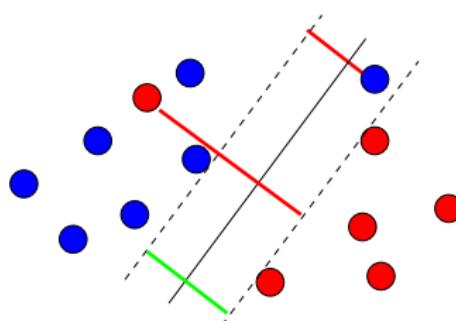
Soft-margin SVM formulation

- The **margin** of a labeled point (x, y) is

$$\text{margin}(x, y) = y \left(w^\top x + b \right)$$

- The **error** is
 - 0 if $\text{margin}(x, y) > 1$,
 - $1 - \text{margin}(x, y)$ otherwise.
- The soft margin SVM solves:

$$\min_{w,b} \left\{ \frac{1}{2} \|w\|^2 + C \sum_{i=1}^n \max \left(0, 1 - y_i (w^\top x_i + b) \right) \right\}$$

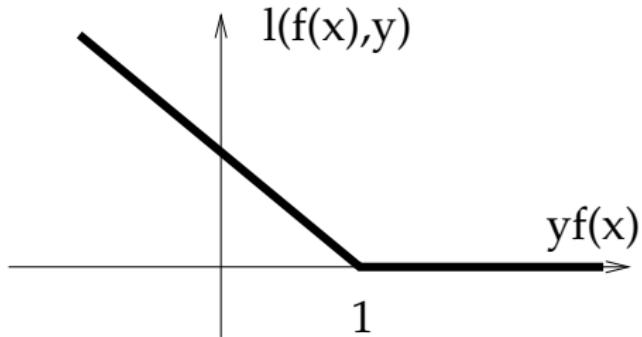
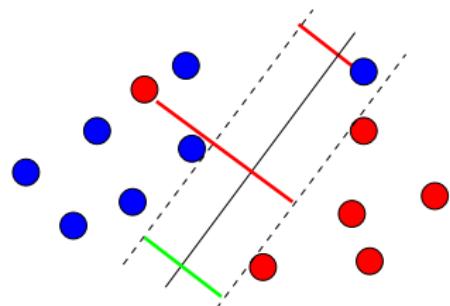


Soft-margin SVM and hinge loss

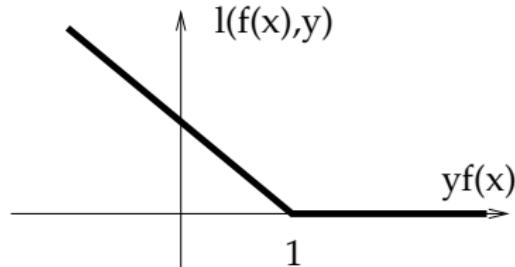
$$\min_{w,b} \left\{ \frac{1}{n} \sum_{i=1}^n \ell_{\text{hinge}}(w^\top x_i + b, y_i) + \lambda \|w\|^2 \right\},$$

for $\lambda = 1/2nC$ and the hinge loss function:

$$\ell_{\text{hinge}}(u, y) = \max(1 - yu, 0) = \begin{cases} 0 & \text{if } yu \geq 1, \\ 1 - yu & \text{otherwise.} \end{cases}$$



Reformulation as a QP



- Note that for any $u \in \mathbb{R}$,

$$\varphi_{\text{hinge}}(u) = \min_{\xi \in \mathbb{R}} \xi \quad \text{such that} \quad \begin{cases} \xi \geq 0 \\ \xi \geq 1 - u \end{cases}$$

- Therefore SVM solves the QP

$$\min_{w, b, \xi} \left\{ \frac{1}{2} \|w\|^2 + C \sum_{i=1}^n \xi_i \right\}, \text{ s.t. } \forall i \in [1, n], \begin{cases} \xi_i \geq 0 \\ \xi_i \geq 1 - y_i (w^\top x_i + b) \end{cases}$$

Lagrangian

Form the Lagrangian:

$$L(w, b, \xi, \alpha, \gamma) = \frac{1}{2} \|w\|^2 + C \sum_{i=1}^n \xi_i - \sum_{i=1}^n \alpha_i (y_i(x_i^\top w + b) + \xi_i - 1) - \gamma^\top \xi$$

Minimize in the primal variables (w, b, ξ) :

$$\nabla_w L = w - \sum_{i=1}^n \alpha_i y_i x_i \implies w = \sum_{i=1}^n \alpha_i y_i x_i$$

$$\nabla_b L = - \sum_{i=1}^n \alpha_i y_i \implies \sum_{i=1}^n \alpha_i y_i = 0$$

$$\nabla_{\xi_i} L = C - \alpha_i - \gamma_i \implies \alpha_i + \gamma_i = C, \forall i \in [1, n]$$

Dual function

- We therefore obtain the **Lagrange dual function**:

$$q(\alpha; \gamma) = \inf_{w \in \mathbb{R}^p, b \in \mathbb{R}} L(w, b, \alpha, \gamma)$$
$$= \begin{cases} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n y_i y_j \alpha_i \alpha_j x_i \cdot x_j & \text{if } \sum_{i=1}^n \alpha_i y_i = 0 \\ & \text{and } \alpha_i + \gamma_i = C, \forall i, \\ -\infty & \text{otherwise.} \end{cases}$$

- The dual problem is:

$$\begin{aligned} & \text{maximize} && q(\alpha, \gamma) \\ & \text{subject to} && \alpha \geq 0 \text{ and } \gamma \geq 0. \end{aligned}$$

- Since γ only appears in the constraints, this is equivalent to maximizing the dual function in α under the constraint $0 \leq \alpha \leq C$

Dual formulation

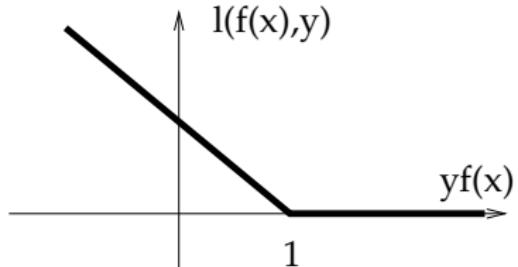
$$\max_{\alpha \in \mathbb{R}^n} \left\{ \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j x_i^\top x_j \right\}$$

under the constraints:

$$\begin{cases} 0 \leq \alpha_i \leq C, & \text{for } i = 1, \dots, n \\ \sum_{i=1}^n \alpha_i y_i = 0. \end{cases}$$

Remark: we recover hard-margin SVM with $C = +\infty$

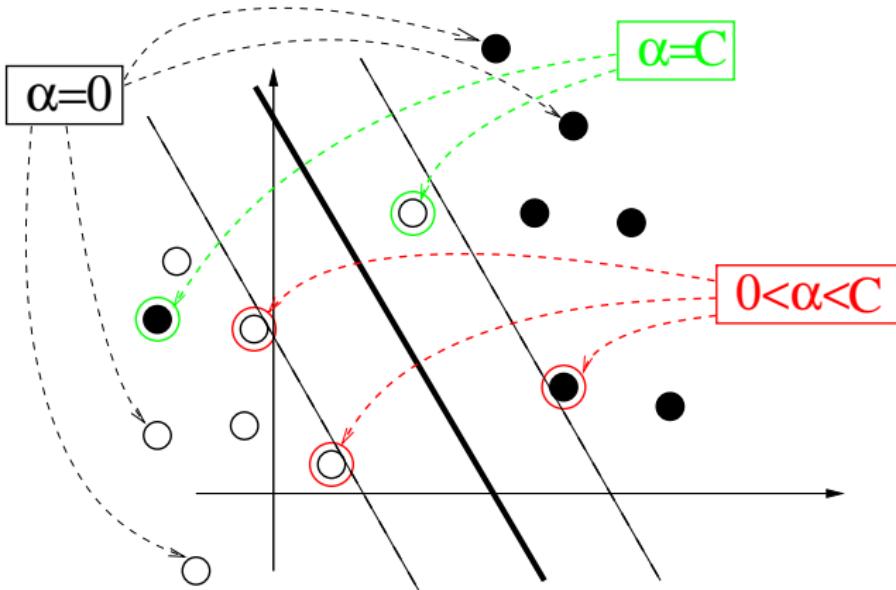
KKT



Let $m_i = y_i(w^\top x_i + b)$ be the margin of the i -th point

- $\alpha_i = 0 \implies \gamma_i > 0 \implies \varphi_{\text{hinge}}(m_i) = 0 \implies m_i \geq 1$
- $\alpha_i = C > 0 \implies \varphi_{\text{hinge}}(m_i) = 1 - m_i \implies m_i \leq 1$
- $0 < \alpha < C \implies (\alpha_i > 0 \text{ and } \gamma_i > 0) \implies \varphi_{\text{hinge}}(m_i) = 1 - m_i = 0 \implies m_i = 1$

Interpretation: bounded and unbounded support vectors



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Loss functions for classifications

We already saw 3 loss functions for binary classification problems

- The 0/1 loss $\ell_{0/1}(f(x), y) = \mathbf{1}(yf(x) < 0)$
- The logistic loss $\ell_{logistic}(f(x), y) = \ln(1 + e^{-yf(x)})$
- The hinge loss $\ell_{hinge}(f(x), y) = \max(0, 1 - yf(x))$

Definition

In binary classification ($\mathcal{Y} = \{-1, 1\}$), the **margin** of the function f for a pair (x, y) is:

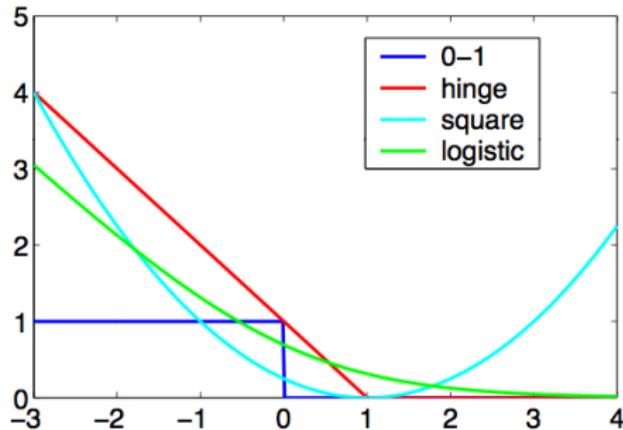
$$yf(x).$$

In all cases the loss is a decreasing function of the margin, i.e.,

$$\ell(f(x), y) = \varphi(yf(x)), \quad \text{with } \varphi \text{ non-increasing}$$

What about other similar loss functions?

Loss function examples



Method	$\varphi(u)$
Logistic regression	$\log(1 + e^{-u})$
Support vector machine (1-SVM)	$\max(1 - u, 0)$
Support vector machine (2-SVM)	$\max(1 - u, 0)^2$
Boosting	e^{-u}

Large-margin classifiers

Definition

Given a non-increasing function $\varphi : \mathbb{R} \rightarrow \mathbb{R}_+$, a large-margin linear classifier is an algorithm that estimates a function $f_\beta(x) = \beta^\top x$ by solving

$$\min_{\beta} \frac{1}{n} \sum_{i=1}^n \varphi(y_i f_\beta(x_i)) + \lambda \|\beta\|_2^2$$

Hence, ridge logistic regression and SVM are large-margin classifier, corresponding to $\varphi(u) = \ln(1 + e^{-u})$ and $\varphi(u) = \max(0, 1 - u)$, respectively. Many more are possible.

Questions:

- ① Can we solve the optimization problem for other φ 's?
- ② Is it a good idea to optimize this objective function, if at the end of the day we are interested in the $\ell_{0/1}$ loss, i.e., learning models that make few errors?

Solving large-margin classifiers

$$\min_{\beta} \frac{1}{n} \sum_{i=1}^n \varphi(y_i \beta^\top x_i) + \lambda \|\beta\|_2^2$$

- When φ is convex, this is a strictly convex function of β
- It can then be solved numerically by generic or specific algorithms for **convex optimization**, e.g., Newton's or gradient method
- When **n is large**, stochastic optimization is particularly useful (at each step, only approximate the gradient with one or a batch of examples)

A tiny bit of learning theory

Assumptions and notations

- Let \mathbb{P} be an (unknown) distribution on $\mathcal{X} \times \mathcal{Y}$, and $\eta(x) = \mathbb{P}(Y = 1 | X = x)$ a measurable version of the conditional distribution of Y given X
- Assume the training set $\mathcal{S}_n = (X_i, Y_i)_{i=1,\dots,n}$ are i.i.d. random variables according to \mathbb{P} .
- The **risk** of a classifier $f : \mathcal{X} \rightarrow \mathbb{R}$ is $R(f) = \mathbb{P}(\text{sign}(f(X)) \neq Y)$
- The **Bayes risk** is

$$R^* = \inf_{f \text{ measurable}} R(f)$$

which is attained for $f^*(x) = \eta(x) - 1/2$

- The **empirical risk** of a classifier $f : \mathcal{X} \rightarrow \mathbb{R}$ is

$$R^n(f) = \frac{1}{n} \sum_{i=1}^n \mathbf{1}(\text{sign}(f(X_i)) \neq Y_i)$$

φ -risk

- Let the **empirical φ -risk** be the empirical risk optimized by a large-margin classifier:

$$R_\varphi^n(f) = \frac{1}{n} \sum_{i=1}^n \varphi(Y_i f(X_i))$$

- It is the empirical version of the **φ -risk**

$$R_\varphi(f) = \mathbb{E}[\varphi(Y f(X))]$$

- Can we hope to have a small risk $R(f)$ if we focus instead on the φ -risk $R_\varphi(f)$?

A small φ -risk ensures a small 0/1 risk

Theorem (Bartlett et al., 2003)

Let $\varphi : \mathbb{R} \rightarrow \mathbb{R}_+$ be convex, non-increasing, differentiable at 0 with $\varphi'(0) < 0$. Let $f : \mathcal{X} \rightarrow \mathbb{R}$ measurable such that

$$R_\varphi(f) = \min_{g \text{ measurable}} R_\varphi(g) = R_\varphi^*.$$

Then

$$R(f) = \min_{g \text{ measurable}} R(g) = R^*.$$

Remarks:

- This tells us that, if we know \mathbb{P} , then minimizing the φ -risk is a good idea even if our focus is on the classification error.
- The assumptions on φ can be relaxed; it works for the broader class of *classification-calibrated* loss functions (Bartlett et al., 2003).
- More generally, we can show that if $R_\varphi(f) - R_\varphi^*$ is small, then $R(f) - R^*$ is small too (Bartlett et al., 2003).

A small φ -risk ensures a small 0/1 risk

Proof sketch:

Condition on $X = x$:

$$R_\varphi(f | X = x) = \mathbb{E}[\varphi(Yf(X)) | X = x] = \eta(x)\varphi(f(x)) + (1 - \eta(x))\varphi(-f(x))$$

$$R_\varphi(-f | X = x) = \mathbb{E}[\varphi(-Yf(X)) | X = x] = \eta(x)\varphi(-f(x)) + (1 - \eta(x))\varphi(f(x))$$

Therefore:

$$R_\varphi(f | X = x) - R_\varphi(-f | X = x) = [2\eta(x) - 1] \times [\varphi(f(x)) - \varphi(-f(x))]$$

This must be a.s. ≤ 0 because $R_\varphi(f) \leq R_\varphi(-f)$, which implies:

- if $\eta(x) > \frac{1}{2}$, $\varphi(f(x)) \leq \varphi(-f(x)) \implies f(x) \geq 0$
- if $\eta(x) < \frac{1}{2}$, $\varphi(f(x)) \geq \varphi(-f(x)) \implies f(x) \leq 0$

These inequalities are in fact strict thanks to the assumptions we made on φ (*left as exercice*). \square

Empirical risk minimization (ERM)

To find a function with a small φ -risk, the following is a good candidate:

Definition

The **ERM estimator** on a functional class \mathcal{F} is the solution (when it exists) of:

$$\hat{f}_n = \operatorname{argmin}_{f \in \mathcal{F}} R_\varphi^n(f).$$

Empirical risk minimization (ERM)

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Definition

The **ERM estimator** on a functional class \mathcal{F} is the solution (when it exists) of:

$$\hat{f}_n = \operatorname{argmin}_{f \in \mathcal{F}} R_\varphi^n(f).$$

Questions:

- ① Is $R_\varphi^n(f)$ a good estimate of the true risk $R_\varphi(f)$?
- ② Is $R_\varphi(\hat{f}_n)$ small?

Class capacity

Motivations

- The ERM principle gives a good solution if $R_\varphi(\hat{f}_n)$ is similar to the minimum achievable risk $\inf_{f \in \mathcal{F}} R_\varphi(f)$.
- This can be ensured if \mathcal{F} is not “too large”.
- We need a measure of the “capacity” of \mathcal{F} .

Definition: Rademacher complexity

The **Rademacher complexity** of a class of functions \mathcal{F} is:

$$\text{Rad}_n(\mathcal{F}) = \mathbb{E}_{X,\sigma} \left[\sup_{f \in \mathcal{F}} \left| \frac{2}{n} \sum_{i=1}^n \sigma_i f(X_i) \right| \right],$$

where the expectation is over $(X_i)_{i=1,\dots,n}$ and the independent uniform $\{\pm 1\}$ -valued (Rademacher) random variables $(\sigma_i)_{i=1,\dots,n}$.

Basic learning bounds

Theorem

Suppose φ is **Lipschitz** with constant L_φ :

$$\forall u, u' \in \mathbb{R}, \quad |\varphi(u) - \varphi(u')| \leq L_\varphi |u - u'|.$$

Then the φ -risk of the ERM estimator satisfies (on average over the sampling of training set)

$$\underbrace{\mathbb{E}_{\mathcal{S}_n} R_\varphi(\hat{f}_n) - R_\varphi^*}_{\text{Excess } \varphi\text{-risk}} \leq \underbrace{4L_\varphi \text{Rad}_n(\mathcal{F})}_{\text{Estimation error}} + \underbrace{\inf_{f \in \mathcal{F}} R_\varphi(f) - R_\varphi^*}_{\text{Approximation error}}$$

This quantifies a trade-off between:

- \mathcal{F} "large" = **overfitting** (approximation error small, estimation error large)
- \mathcal{F} "small" = **underfitting** (estimation error small, approximation error large)

ERM for bounded linear classifiers

Consider the set of linear functions $f_\beta(x) = \beta^\top x$ where β is bounded:

$$\mathcal{F}_B = \{f_\beta : \|\beta\|_2 \leq B\}.$$

Theorem

$$\text{Rad}_n(\mathcal{F}_B) \leq \frac{2B\sqrt{\mathbb{E}\|X\|_2^2}}{\sqrt{n}}.$$

Proof (1/2)

$$\begin{aligned}
 \text{Rad}_n(\mathcal{F}_B) &= \mathbb{E}_{X,\sigma} \left[\sup_{f \in \mathcal{F}_B} \left| \frac{2}{n} \sum_{i=1}^n \sigma_i f(X_i) \right| \right] \\
 &= \mathbb{E}_{X,\sigma} \left[\sup_{\|\beta\| \leq B} \left| \left\langle \beta, \frac{2}{n} \sum_{i=1}^n \sigma_i X_i \right\rangle \right| \right] \quad (\text{linearity}) \\
 &= \mathbb{E}_{X,\sigma} \left[B \left\| \frac{2}{n} \sum_{i=1}^n \sigma_i X_i \right\|_2 \right] \quad (\text{Cauchy-Schwarz}) \\
 &= \frac{2B}{n} \mathbb{E}_{X,\sigma} \left[\sqrt{\left\| \sum_{i=1}^n \sigma_i X_i \right\|_2^2} \right] \\
 &\leq \frac{2B}{n} \sqrt{\mathbb{E}_{X,\sigma} \left[\sum_{i,j=1}^n \sigma_i \sigma_j X_i^\top X_j \right]} \quad (\text{Jensen})
 \end{aligned}$$

Proof (2/2)

But $\mathbb{E}_\sigma [\sigma_i \sigma_j]$ is 1 if $i = j$, 0 otherwise. Therefore:

$$\begin{aligned}\text{Rad}_n(\mathcal{F}_B) &\leq \frac{2B}{n} \sqrt{\mathbb{E}_X \left[\sum_{i,j=1}^n \mathbb{E}_\sigma [\sigma_i \sigma_j] X_i^\top X_j \right]} \\ &\leq \frac{2B}{n} \sqrt{\mathbb{E}_X \sum_{i=1}^n \|X_i\|_2^2} \\ &= \frac{2B \sqrt{\mathbb{E}_X \|X\|_2^2}}{\sqrt{n}}.\quad \square\end{aligned}$$

Basic learning bounds in RKHS balls

Corollary

Suppose $\|X\| \leq \kappa$ a.s. Then the ERM estimator in \mathcal{F}_B satisfies

$$\mathbb{E}R_\varphi(\hat{f}_n) - R_\varphi^* \leq \frac{8L_\varphi\kappa B}{\sqrt{n}} + \left[\inf_{f \in \mathcal{F}_B} R_\varphi(f) - R_\varphi^* \right].$$

Remarks

- B controls the trade-off between approximation and estimation error
- The bound on expression error is independent of \mathcal{P} and decreases with n
- The approximation error is harder to analyze in general
- In practice, B (or λ , next slide) is tuned by cross-validation

ERM as penalized risk minimization

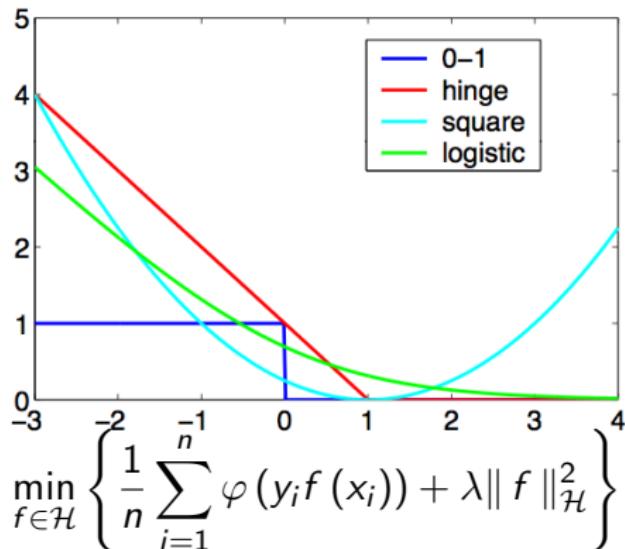
- ERM over \mathcal{F}_B solves the **constrained minimization problem**:

$$\begin{cases} \min_{\beta} \frac{1}{n} \sum_{i=1}^n \varphi(y_i; f_\beta(x_i)) \\ \text{subject to } \|\beta\|_2 \leq B. \end{cases}$$

- To make this practical we assume that φ is **convex**.
- The problem is then a **convex problem** in β for which **strong duality holds**. In particular β solves the problem if and only if it solves for some dual parameter λ the **unconstrained problem**:

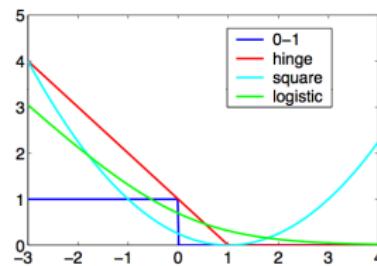
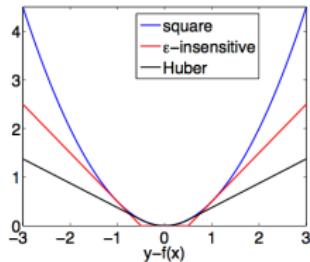
$$\min_{\beta \in \mathbb{R}^p} \left\{ \frac{1}{n} \sum_{i=1}^n \varphi(y_i; f_\beta(x_i)) + \lambda \|\beta\|_2^2 \right\}.$$

Summary: large margin classifiers



- φ calibrated (e.g., decreasing, $\varphi'(0) < 0$) \implies good proxy for classification error
- φ convex + representer theorem \implies efficient algorithms

Summary: ℓ_2 -regularized linear methods



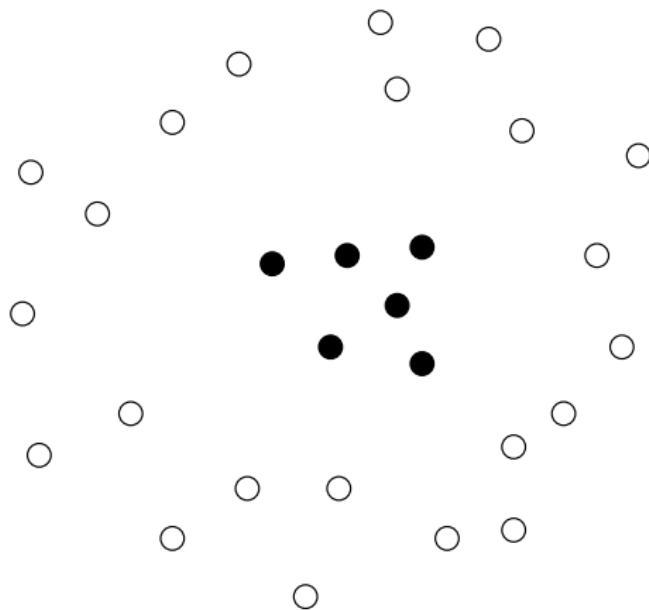
$$f_{\beta}(x) = \beta^\top x, \quad \min_{\beta} \left\{ \frac{1}{n} \sum_{i=1}^n \ell(f_{\beta}(x_i), y_i) + \lambda \|\beta\|_2^2 \right\}$$

- Many popular methods for regression and classification are obtained by changing the loss function: ridge regression, logistic regression, SVM...
- Needs to solve numerically a convex optimization problem, well adapted to large datasets (stochastic gradient...)
- In practice, very similar performance between the different variants in general

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Motivation

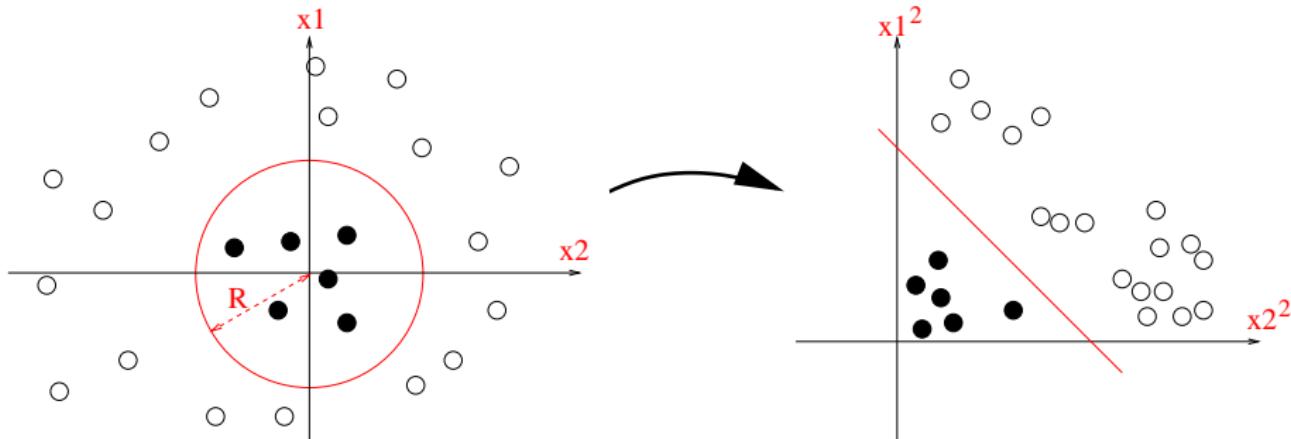


- Sometimes linear models are not interesting...
- Kernels will allow to solve nonlinear problems with linear methods!

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"Linear" depends on the representation you choose



For $x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$ let $\Phi(x) = \begin{pmatrix} x_1^2 \\ x_2^2 \end{pmatrix}$. The decision function is:

$$f(x) = x_1^2 + x_2^2 - R^2 = \beta^\top \Phi(x) + b$$

with $\beta = (1, 1)^\top$ and $b = -R^2$

Kernel = inner product in the feature space

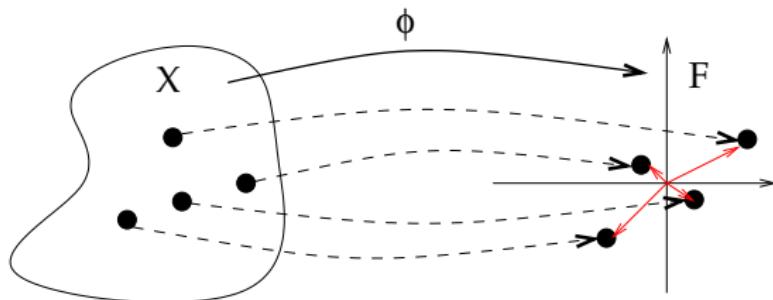
Definition

For a given mapping

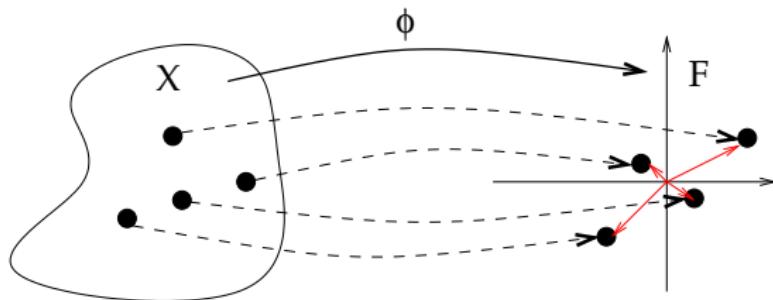
$$\Phi : \mathcal{X} \mapsto \mathcal{H}$$

from the space of data \mathcal{X} to some feature space \mathcal{H} , the **kernel** between two objects x and x' is the inner product of their images:

$$\forall x, x' \in \mathcal{X}, \quad K(x, x') = \Phi(x)^\top \Phi(x').$$



Example

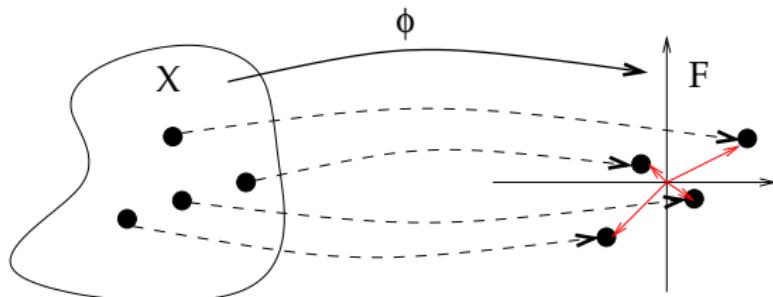


Let $\mathcal{X} = \mathcal{H} = \mathbb{R}^2$ and for $x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$ let $\Phi(x) = \begin{pmatrix} x_1^2 \\ x_2^2 \end{pmatrix}$

Then the kernel is:

$$K(x, x') = \Phi(x)^\top \Phi(x') = (x_1)^2 (x'_1)^2 + (x_2)^2 (x'_2)^2.$$

The kernel tricks



2 tricks

- ① Many linear algorithms (in particular ℓ_2 -regularized methods) can be performed in the feature space of $\Phi(x)$ without explicitly computing the images $\Phi(x)$, but instead by computing kernels $K(x, x')$.
- ② It is sometimes possible to easily compute kernels which correspond to complex large-dimensional feature spaces: $K(x, x')$ is often much simpler to compute than $\Phi(x)$ and $\Phi(x')$

Trick 1 illustration: SVM in the original space

- Train the SVM by maximizing

$$\max_{\alpha \in \mathbb{R}^n} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j \mathbf{x}_i^\top \mathbf{x}_j,$$

under the constraints:

$$\begin{cases} 0 \leq \alpha_i \leq C, & \text{for } i = 1, \dots, n \\ \sum_{i=1}^n \alpha_i y_i = 0. \end{cases}$$

- Predict with the decision function

$$f(\mathbf{x}) = \sum_{i=1}^n \alpha_i y_i \mathbf{x}_i^\top \mathbf{x} + b^*.$$

Trick 1 illustration: SVM in the feature space

- Train the SVM by maximizing

$$\max_{\alpha \in \mathbb{R}^n} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j \Phi(x_i)^\top \Phi(x_j),$$

under the constraints:

$$\begin{cases} 0 \leq \alpha_i \leq C, & \text{for } i = 1, \dots, n \\ \sum_{i=1}^n \alpha_i y_i = 0. \end{cases}$$

- Predict with the decision function

$$f(x) = \sum_{i=1}^n \alpha_i y_i \Phi(x_i)^\top \Phi(x) + b^*.$$

Trick 1 illustration: SVM in the feature space with a kernel

- Train the SVM by maximizing

$$\max_{\alpha \in \mathbb{R}^n} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j K(x_i, x_j),$$

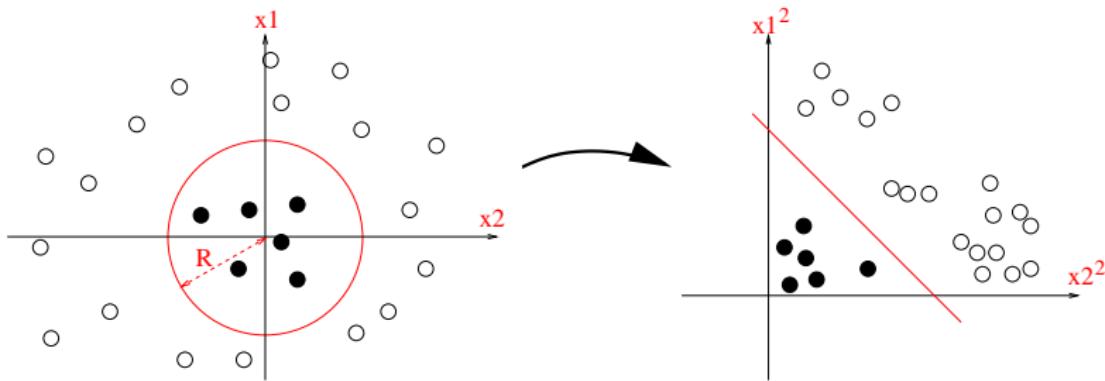
under the constraints:

$$\begin{cases} 0 \leq \alpha_i \leq C, & \text{for } i = 1, \dots, n \\ \sum_{i=1}^n \alpha_i y_i = 0. \end{cases}$$

- Predict with the decision function

$$f(x) = \sum_{i=1}^n \alpha_i y_i K(x_i, x) + b^*.$$

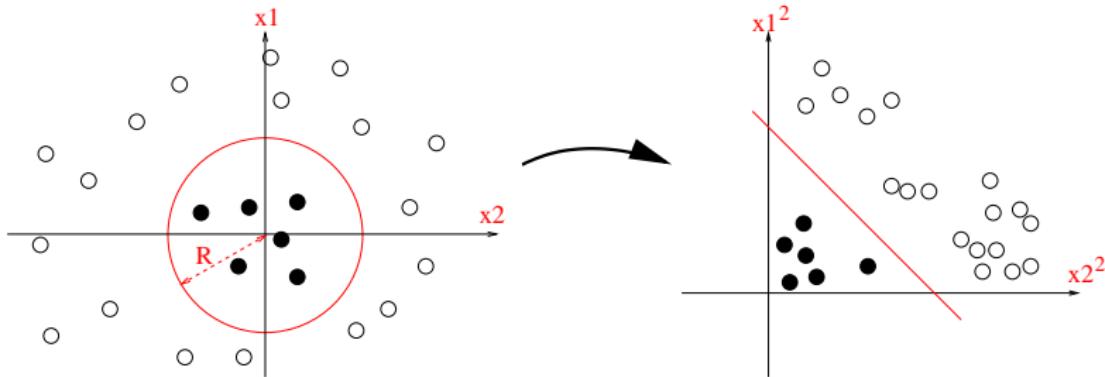
Trick 2 illustration: polynomial kernel



For $x = (x_1, x_2)^\top \in \mathbb{R}^2$, let $\Phi(x) = (x_1^2, \sqrt{2}x_1x_2, x_2^2) \in \mathbb{R}^3$:

$$\begin{aligned} K(x, x') &= x_1^2 x'^2 + 2x_1 x_2 x'_1 x'_2 + x_2^2 x'^2 \\ &= (x_1 x'_1 + x_2 x'_2)^2 \\ &= (x^\top x')^2. \end{aligned}$$

Trick 2 illustration: polynomial kernel



More generally, for $x, x' \in \mathbb{R}^p$,

$$K(x, x') = (x^\top x' + 1)^d$$

is an inner product in a feature space of all monomials of degree up to d
(left as exercise.)

Combining tricks: learn a polynomial discrimination rule with SVM

- Train the SVM by maximizing

$$\max_{\alpha \in \mathbb{R}^n} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j (x_i^\top x_j + 1)^d,$$

under the constraints:

$$\begin{cases} 0 \leq \alpha_i \leq C, & \text{for } i = 1, \dots, n \\ \sum_{i=1}^n \alpha_i y_i = 0. \end{cases}$$

- Predict with the decision function

$$f(x) = \sum_{i=1}^n \alpha_i y_i (x_i^\top x + 1)^d + b^*.$$

Illustration: toy nonlinear problem

```
> plot(x,col=ifelse(y>0,1,2),pch=ifelse(y>0,1,2))
```

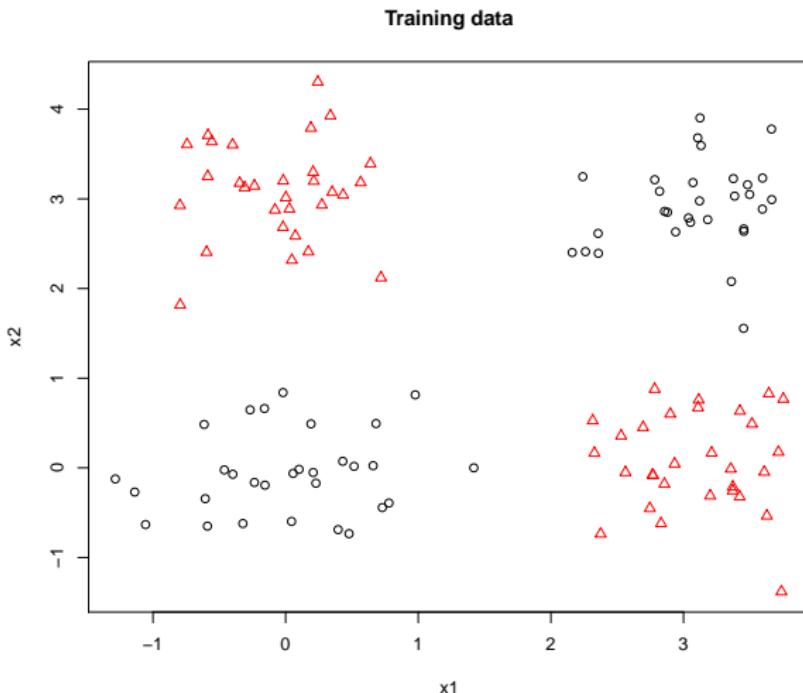


Illustration: toy nonlinear problem, linear SVM

```
> library(kernlab)  
> svp <- ksvm(x,y,type="C-svc",kernel='vanilladot')  
> plot(svp,data=x)
```

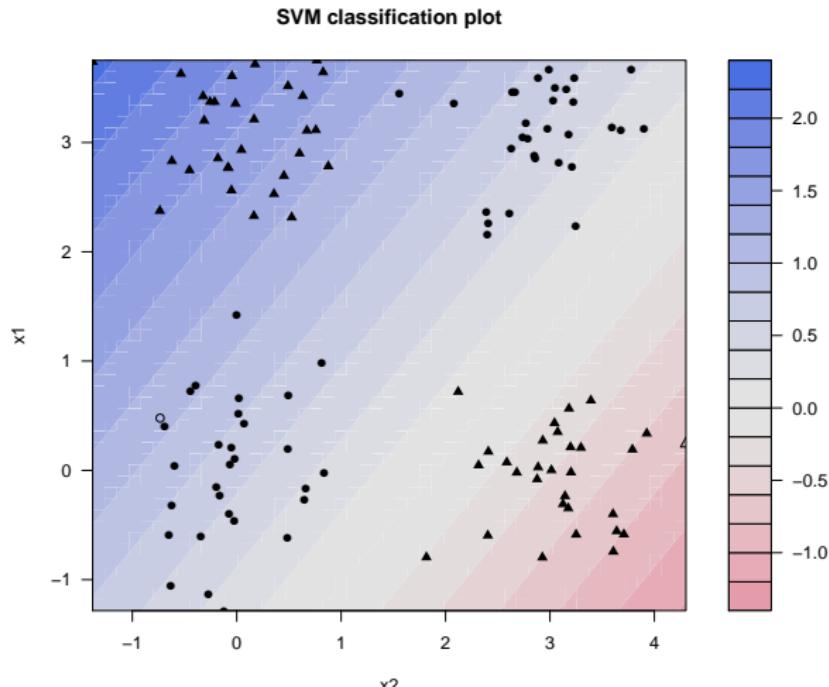
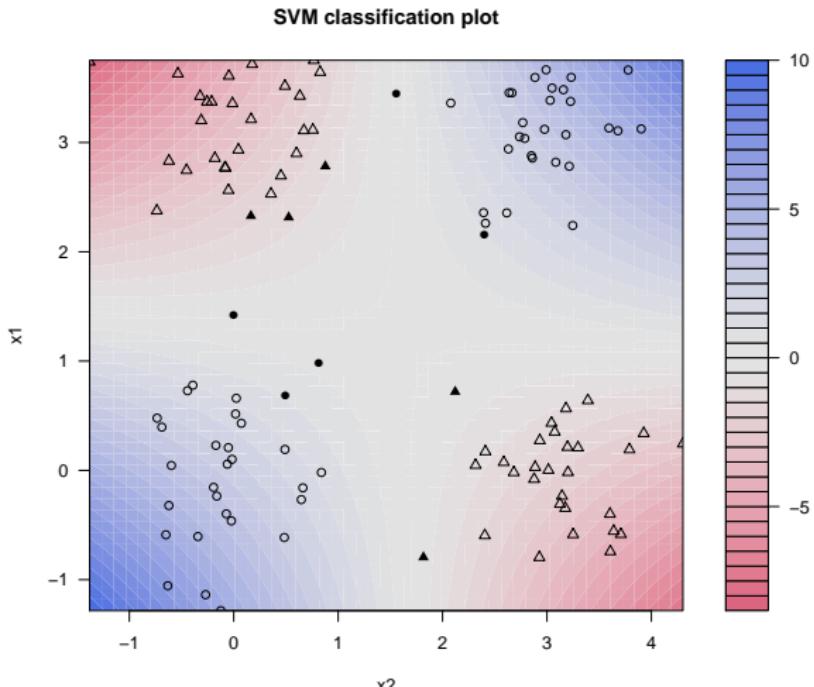


Illustration: toy nonlinear problem, polynomial SVM

```
> svp <- ksvm(x,y,type="C-svc", ...
                 kernel=polydot(degree=2))
> plot(svp,data=x)
```



More generally: trick 1 for ℓ_2 -regularized linear models

Representer theorem

Let $f_\beta(x) = \beta^\top \Phi(x)$. Then any solution \hat{f}_β of

$$\min_{\beta} \frac{1}{n} \sum_{i=1}^n \ell(f_\beta(x_i), y_i) + \lambda \|\beta\|_2^2$$

can be expanded as

$$\hat{f}_\beta(x) = \sum_{i=1}^n \alpha_i K(x_i, x),$$

where $\alpha \in \mathbb{R}^n$ is a solution of:

$$\min_{\alpha \in \mathbb{R}^n} \frac{1}{n} \sum_{i=1}^n \ell \left(\sum_{j=1}^n \alpha_j K(x_i, x_j), y_i \right) + \lambda \sum_{i,j=1}^n \alpha_i \alpha_j K(x_i, x_j).$$

Representer theorem: proof

- For any $\beta \in \mathbb{R}^p$, decompose $\beta = \beta_S + \beta_{\perp}$ where $\beta_S \in \text{span}(\Phi(x_1), \dots, \Phi(x_n))$ and β_{\perp} is orthogonal to it.
- On any point x_i of the training set, we have:

$$f_{\beta}(x_i) = \beta^T \Phi(x_i) = \beta_S^T \Phi(x_i) + \beta_{\perp}^T \Phi(x_i) = \beta_S^T \Phi(x_i) = f_{\beta_S}(x_i).$$

- On the other hand, we have $\|\beta\|_2^2 = \|\beta_S\|_2^2 + \|\beta_{\perp}\|_2^2 \geq \|\beta_S\|_2^2$, with strict inequality if $\beta_{\perp} \neq 0$.
- Consequently, β_S is always as good as β in terms of objective function, and strictly better if $\beta_{\perp} \neq 0$. This implies that at any minimum, $\beta_{\perp} = 0$ and therefore $\beta = \beta_S = \sum_{i=1}^n \alpha_i \Phi(x_i)$ for some $\alpha \in \mathbb{R}^n$.
- We then just replace β by this expression in the objective function, noting that

$$\|\beta\|_2^2 = \left\| \sum_{i=1}^n \alpha_i \Phi(x_i) \right\|_2^2 = \sum_{i,j=1}^n \alpha_i \alpha_j \Phi(x_i)^T \Phi(x_j) = \sum_{i,j=1}^n \alpha_i \alpha_j K(x_i, x_j).$$

Example: kernel ridge regression

- Let $\Phi : \mathcal{X} \rightarrow \mathbb{R}^P$ be a feature mapping from the space of data to a Euclidean or Hilbert space.
- Let $f_\beta(x) = \beta^\top \Phi(x)$ and K the corresponding kernel.
- By the representer theorem, any solution of:

$$\hat{f} = \arg \min_{f_\beta} \frac{1}{n} \sum_{i=1}^n (y_i - f_\beta(x_i))^2 + \lambda \|\beta\|_2^2$$

can be expanded as:

$$\hat{f} = \sum_{i=1}^n \alpha_i K(x_i, x).$$

Example: kernel ridge regression

- Let $Y = (y_1, \dots, y_n)^\top \in \mathbb{R}^n$ the vector of response variables.
- Let $\alpha = (\alpha_1, \dots, \alpha_n)^\top \in \mathbb{R}^n$ the unknown coefficients.
- Let K be the $n \times n$ Gram matrix: $K_{i,j} = K(x_i, x_j)$.
- We can then write in matrix form:

$$(\hat{f}(x_1), \dots, \hat{f}(x_n))^\top = K\alpha,$$

- Moreover,

$$\|\beta\|_2^2 = \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j K(x_i, x_j) = \alpha^\top K \alpha.$$

Example: kernel ridge regression

- The problem is therefore equivalent to:

$$\arg \min_{\alpha \in \mathbb{R}^n} \frac{1}{n} (K\alpha - Y)^\top (K\alpha - Y) + \lambda \alpha^\top K \alpha.$$

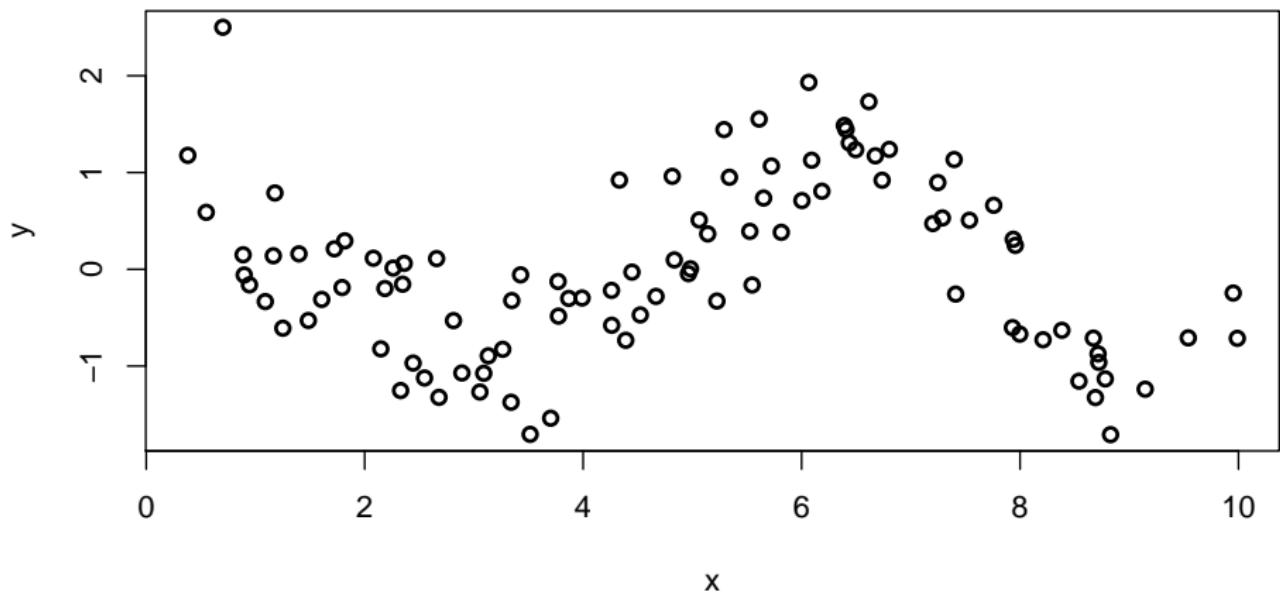
- This is a convex and differentiable function of α . Its minimum can therefore be found by setting the gradient in α to zero:

$$\begin{aligned} 0 &= \frac{2}{n} K(K\alpha - Y) + 2\lambda K\alpha \\ &= K[(K + \lambda n I)\alpha - Y] \end{aligned}$$

- For $\lambda > 0$, $K + \lambda n I$ is invertible (because K is positive semidefinite) so one solution is to take:

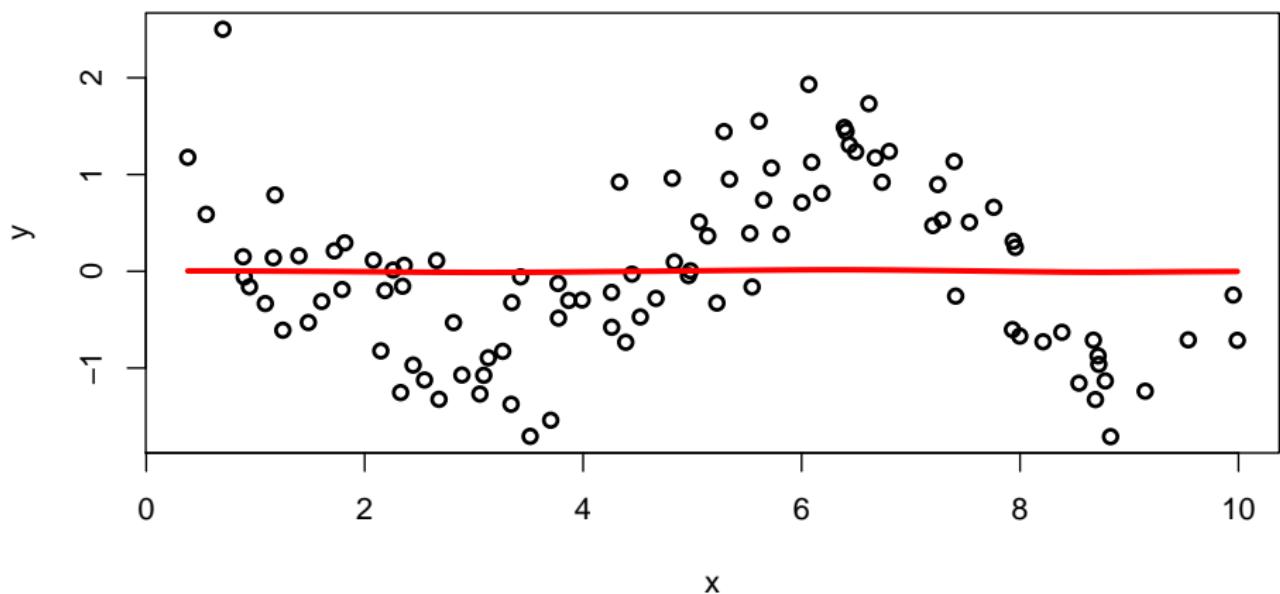
$$\alpha = (K + \lambda n I)^{-1} Y.$$

Example (KRR with Gaussian RBF kernel)



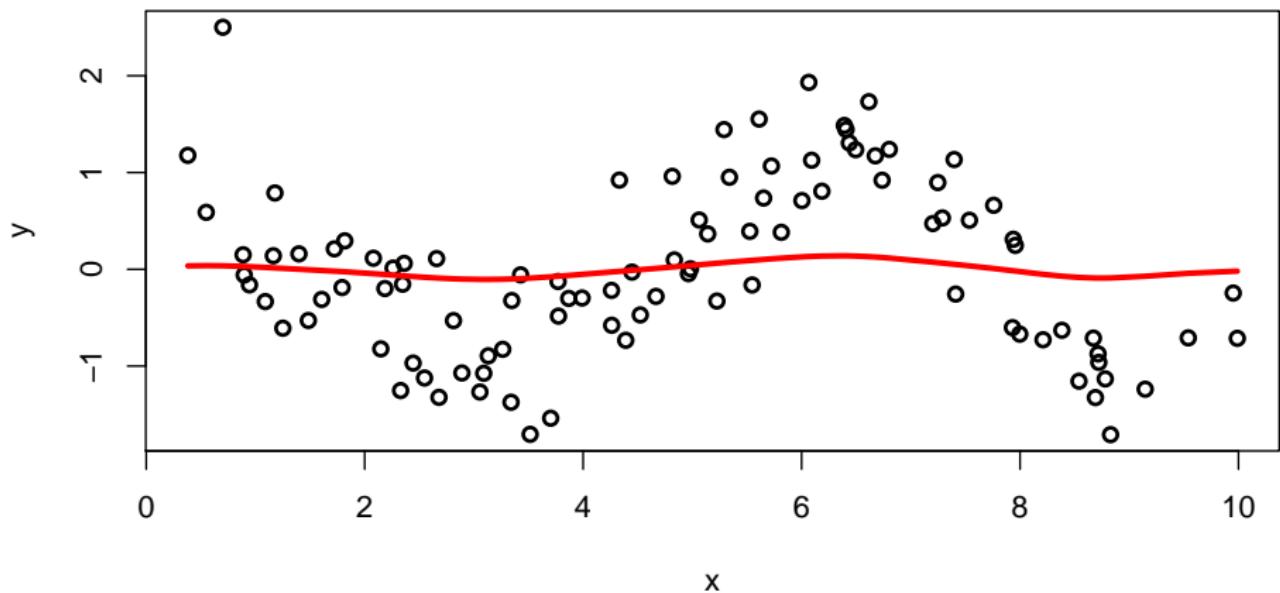
Example (KRR with Gaussian RBF kernel)

lambda = 1000



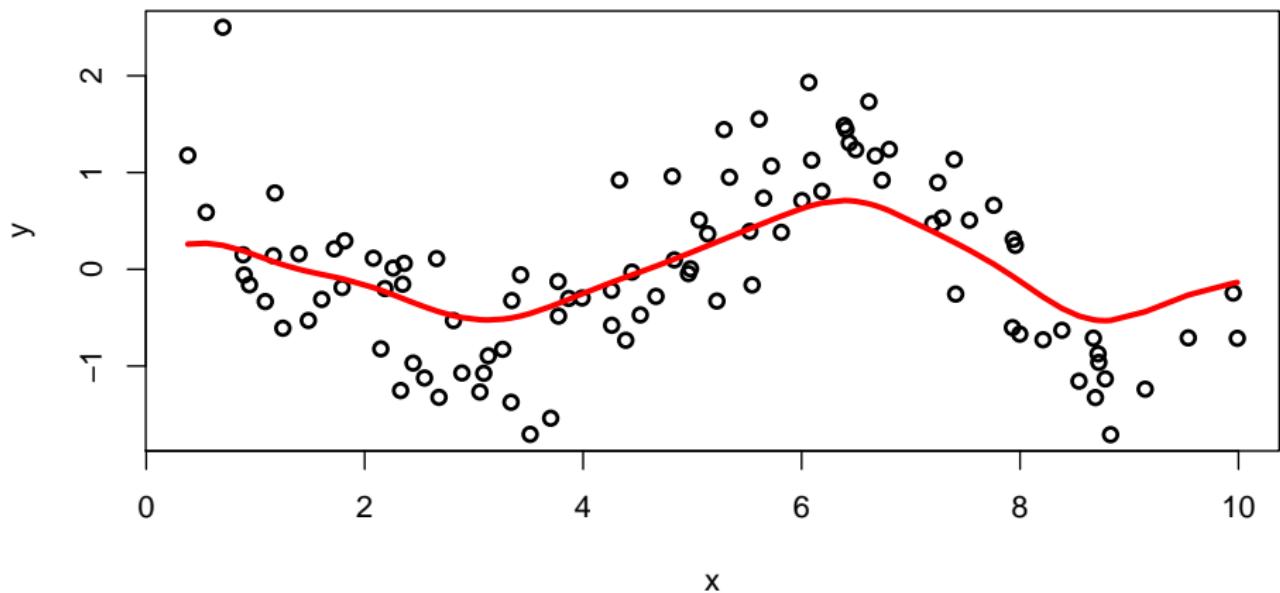
Example (KRR with Gaussian RBF kernel)

lambda = 100



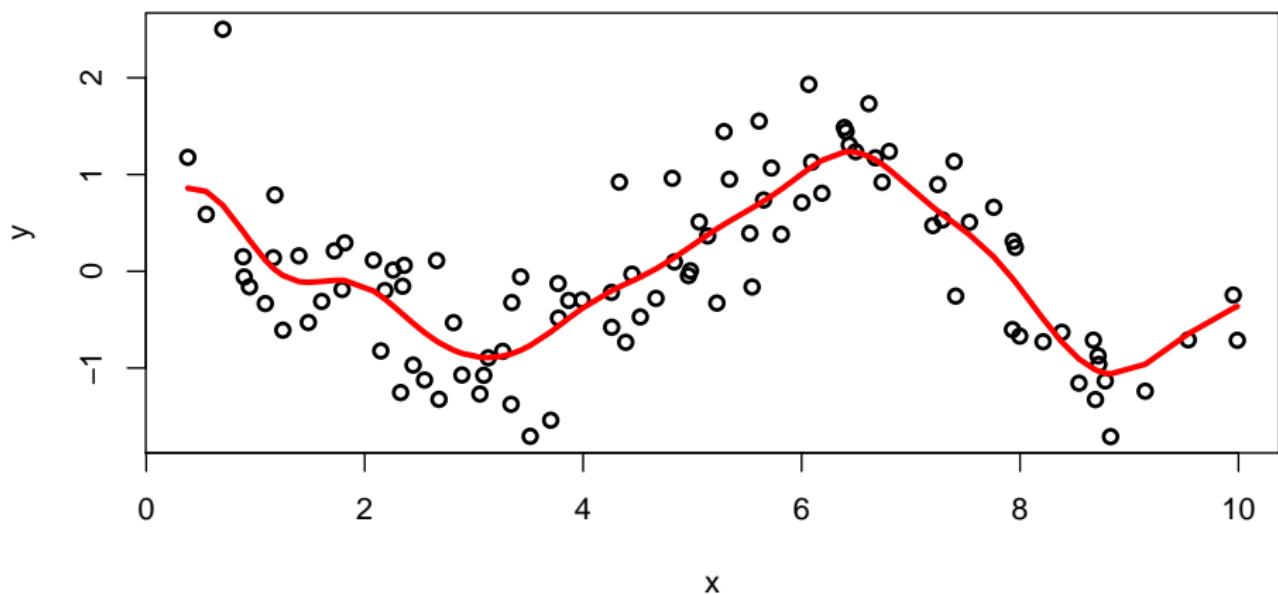
Example (KRR with Gaussian RBF kernel)

lambda = 10



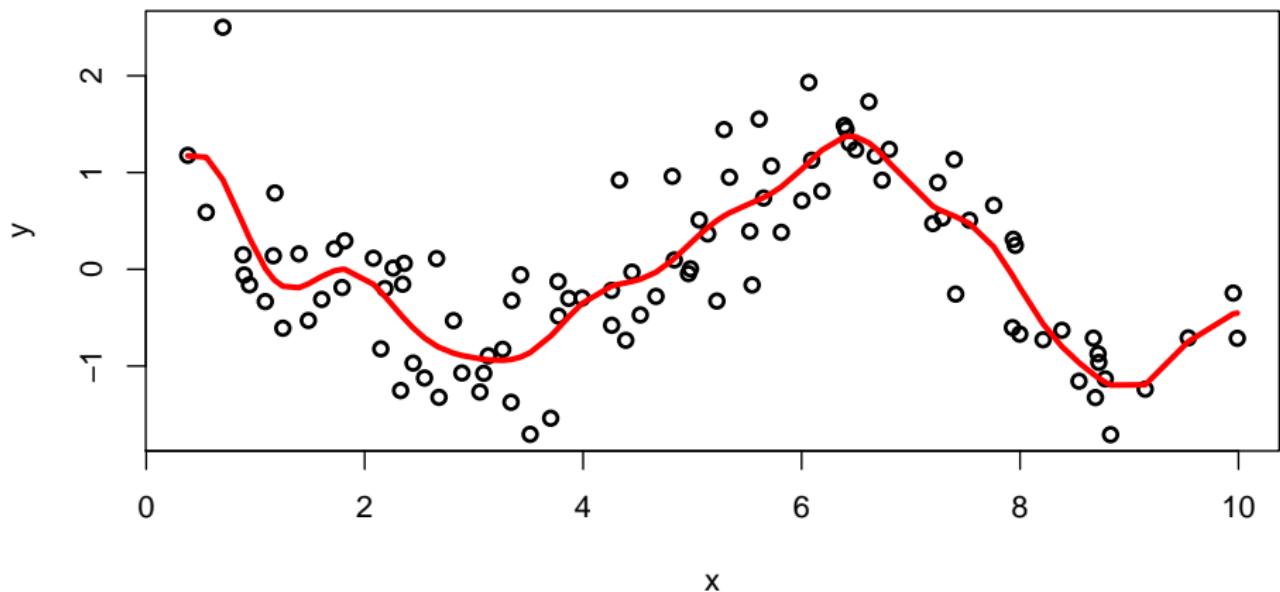
Example (KRR with Gaussian RBF kernel)

lambda = 1



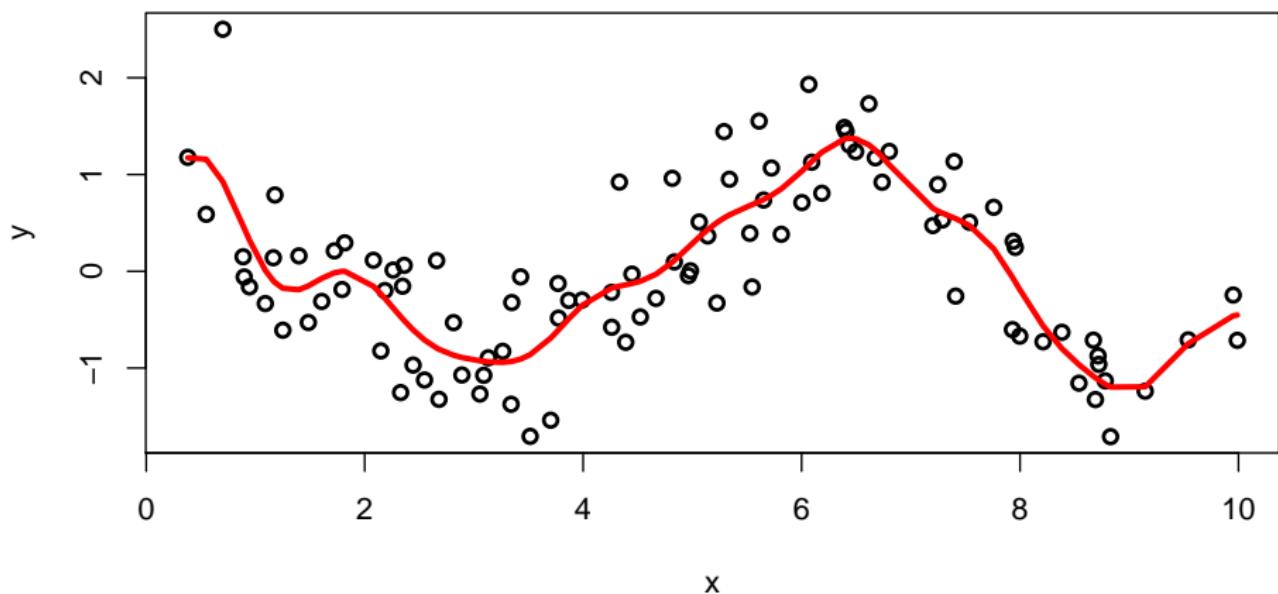
Example (KRR with Gaussian RBF kernel)

lambda = 0.1



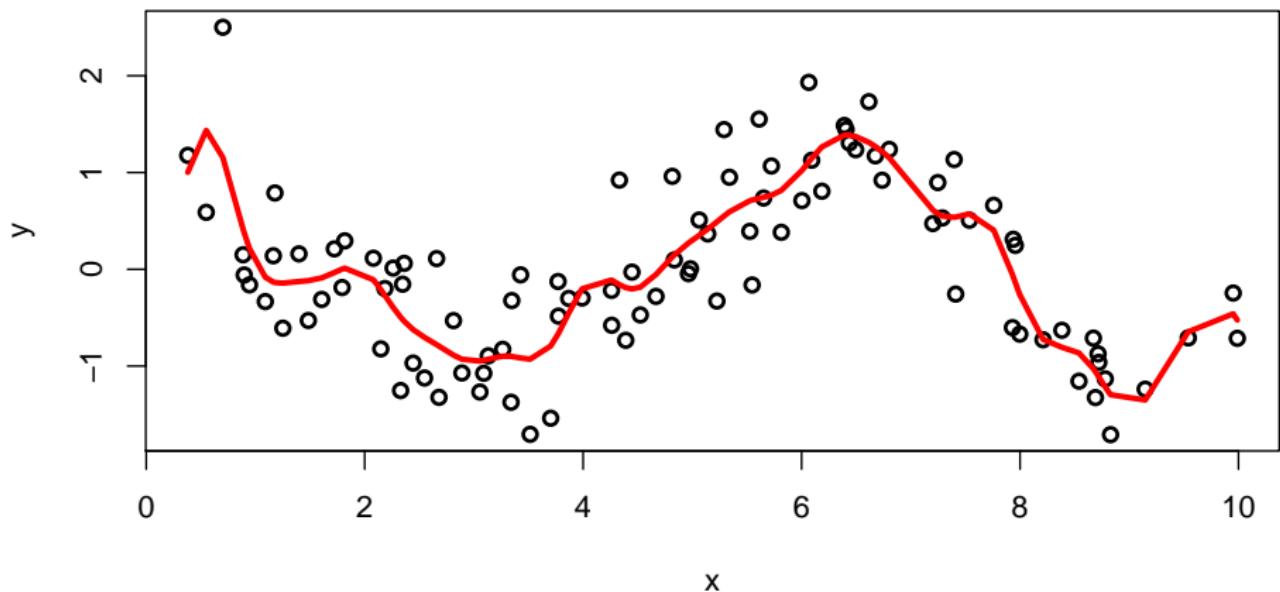
Example (KRR with Gaussian RBF kernel)

lambda = 0.01



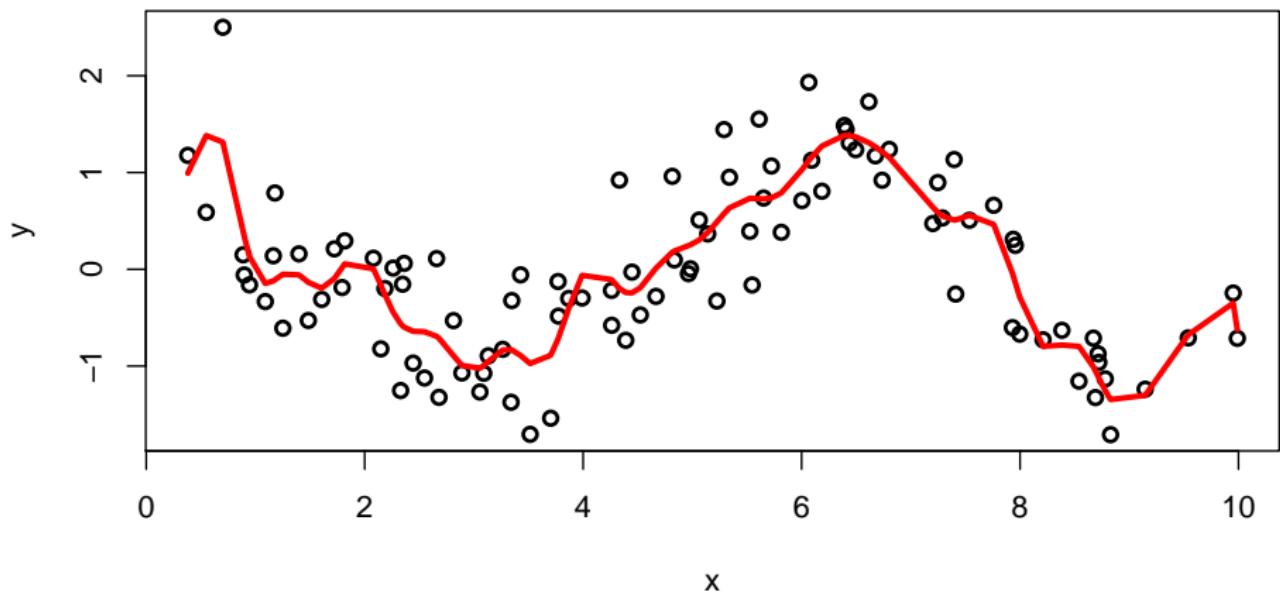
Example (KRR with Gaussian RBF kernel)

lambda = 0.001



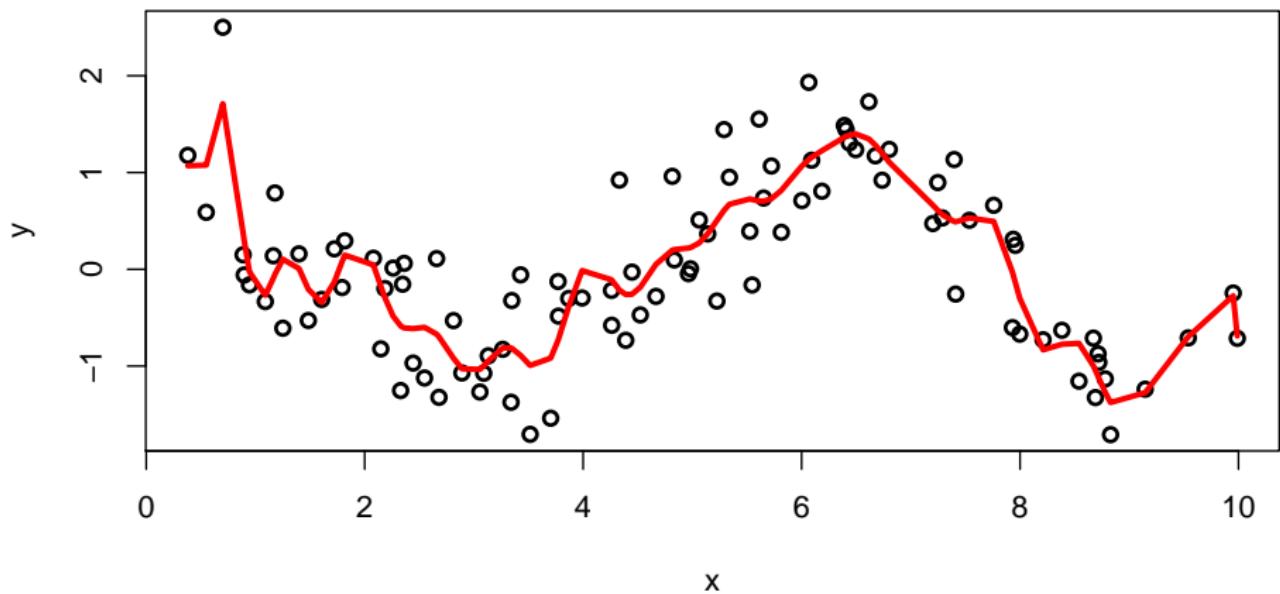
Example (KRR with Gaussian RBF kernel)

lambda = 0.0001



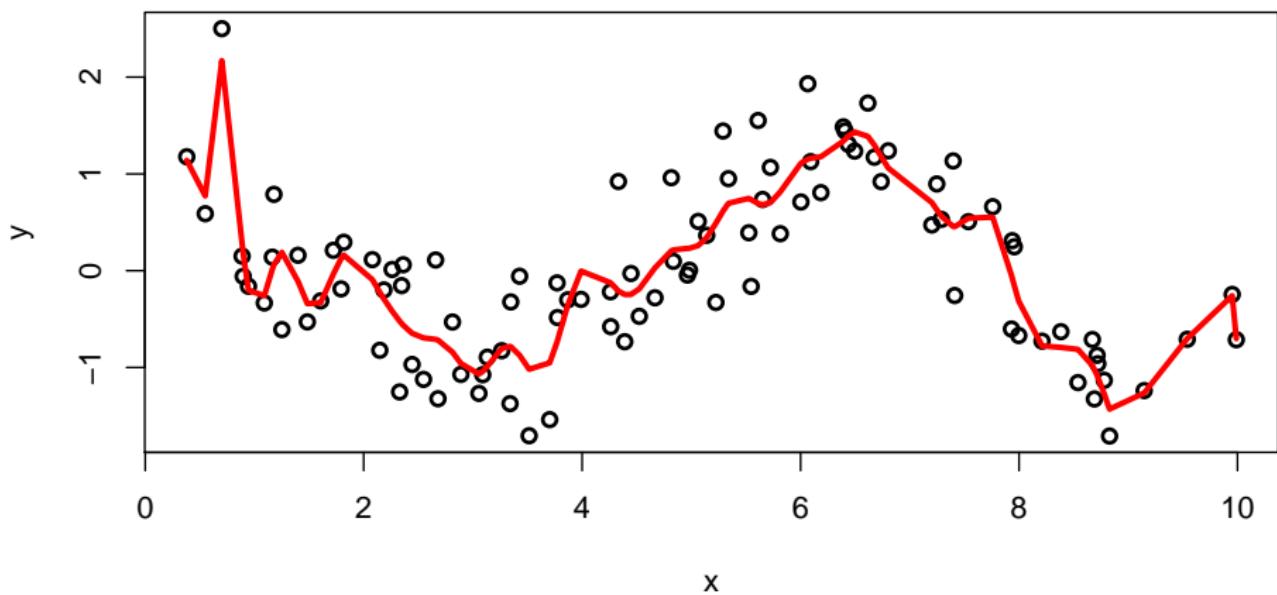
Example (KRR with Gaussian RBF kernel)

lambda = 0.00001



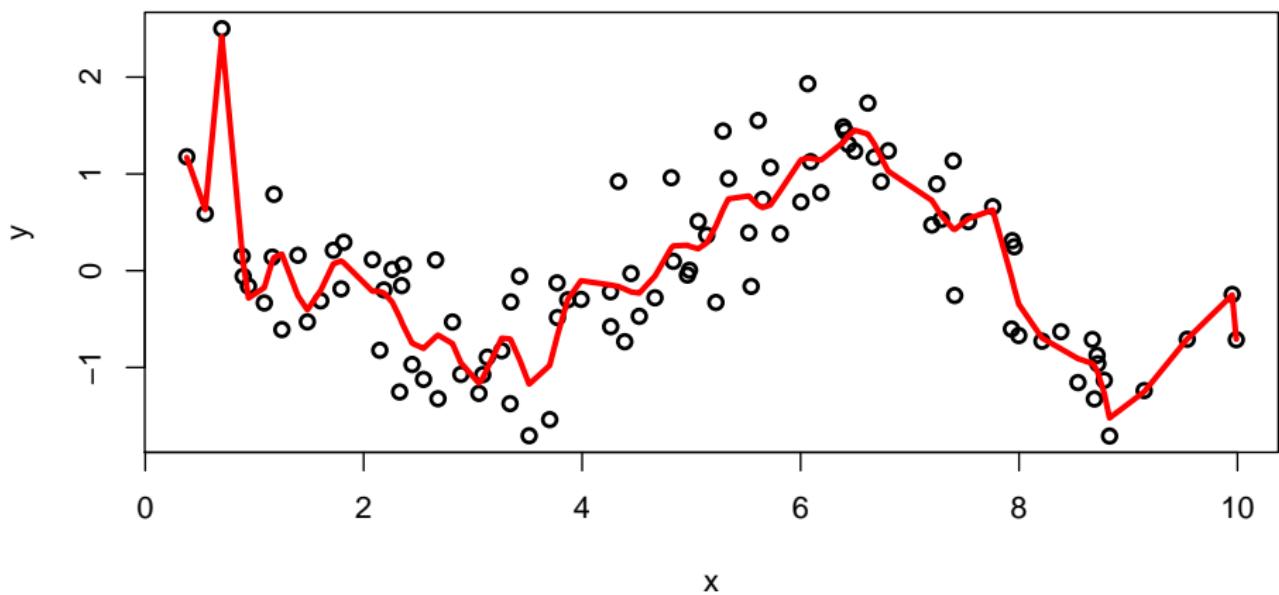
Example (KRR with Gaussian RBF kernel)

lambda = 0.000001



Example (KRR with Gaussian RBF kernel)

lambda = 0.0000001



Remark: uniqueness of the solution

Let us find *all* α 's that solve

$$K[(K + \lambda nI)\alpha - Y] = 0$$

- K being a symmetric matrix, it can be diagonalized in an orthonormal basis and $\text{Ker}(K) \perp \text{Im}(K)$.
- In this basis we see that $(K + \lambda nI)^{-1}$ leaves $\text{Im}(K)$ and $\text{Ker}(K)$ invariant.
- The problem is therefore equivalent to:

$$\begin{aligned} & (K + \lambda nI)\alpha - Y \in \text{Ker}(K) \\ \Leftrightarrow & \alpha - (K + \lambda nI)^{-1}Y \in \text{Ker}(K) \\ \Leftrightarrow & \alpha = (K + \lambda nI)^{-1}Y + \epsilon, \text{ with } K\epsilon = 0. \end{aligned}$$

- However, if $\alpha' = \alpha + \epsilon$ with $K\epsilon = 0$, then:

$$\|\beta - \beta'\|_2^2 = (\alpha - \alpha')^\top K (\alpha - \alpha') = 0,$$

therefore $\beta = \beta'$. KRR has a unique solution β , which can possibly be expressed by several α 's if K is singular.

Comparison with "standard" ridge regression

- Let X the $n \times p$ data matrix, $K = XX^\top$ the kernel Gram matrix.
- In "standard" ridge regression, we have $\hat{f}(x) = \hat{\beta}^\top x$ with

$$\hat{\beta} = (X^\top X + n\lambda I)^{-1} X^\top Y.$$

- In "kernel" ridge regression, we have $\tilde{f}(x) = \sum_{i=1}^n \alpha_i x_i^\top x = \tilde{\beta}^\top x$ with

$$\tilde{\beta} = \sum_{i=1}^n \alpha_i x_i = X^\top \alpha = X^\top (X X^\top + \lambda n I)^{-1} Y.$$

- Oups... which one is correct?

Comparison with "standard" ridge regression

Matrix inversion lemma

For any matrices B and C , and $\gamma > 0$ the following holds (when it makes sense):

$$B(CB + \gamma I)^{-1} = (BC + \gamma I)^{-1}B$$

We deduce that (of course...):

$$\hat{\beta} = \underbrace{(X^\top X + n\lambda I)^{-1}}_{p \times p} X^\top Y = X^\top \underbrace{(XX^\top + \lambda nI)^{-1}}_{n \times n} Y = \tilde{\beta}$$

Computationally, inverting the matrix is the expensive part, which suggest to implement:

- KRR when $p > n$ (high dimension)
- RR when $p < n$ (many points)

Generalization

- We learn the function $f(x) = \sum_{i=1}^n \alpha_i K(x_i, x)$ by solving in α the following optimization problem, with adequate loss function ℓ :

$$\min_{\alpha \in \mathbb{R}^n} \frac{1}{n} \sum_{i=1}^n \ell \left(\sum_{j=1}^n \alpha_j K(x_i, x_j), y_i \right) + \lambda \sum_{i,j=1}^n \alpha_i \alpha_j K(x_i, x_j).$$

- No explicit solution, but **convex** optimization problem
- Note that the **dimension** of the problem is now n instead of p (useful when $n < p$)

The case of SVM

- Soft-margin SVM with a kernel solves:

$$\min_{\alpha \in \mathbb{R}^n, b \in \mathbb{R}} \left\{ \sum_{i=1}^n \ell_{\text{hinge}} \left(\sum_{j=1}^n \alpha_j K(x_i, x_j), y_i \right) + \lambda \sum_{i,j=1}^n \alpha_i \alpha_j K(x_i, x_j) \right\}.$$

- By Lagrange duality we saw that this is equivalent to

$$\max_{\alpha \in \mathbb{R}^n} L(\alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j K(x_i, x_j) + b,$$

under the constraints:

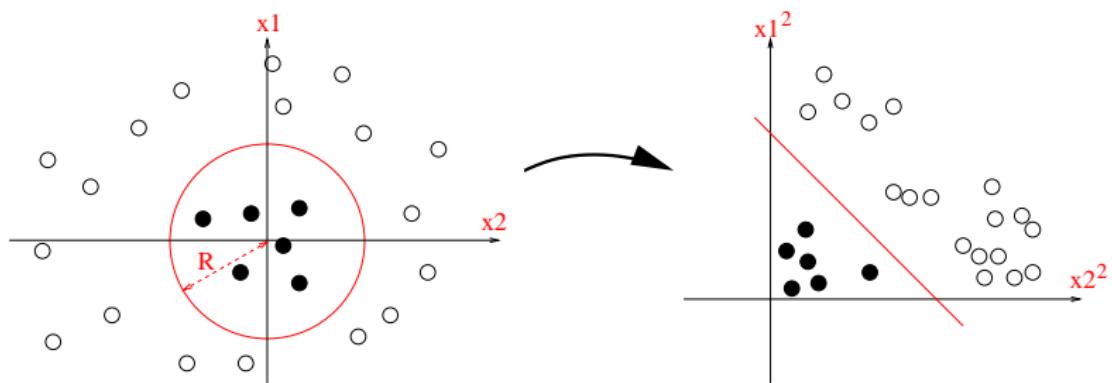
$$\begin{cases} 0 \leq \alpha_i \leq C, & \text{for } i = 1, \dots, n \\ \sum_{i=1}^n \alpha_i y_i = 0. \end{cases}$$

- This is not a surprise, both problems are also dual to each other (*exercise*).

Outline

- 1 Learning in high dimension
- 2 Learning with ℓ_2 regularization
 - Ridge regression
 - Ridge logistic regression
 - Linear hard-margin SVM
 - Interlude: quick notes on constrained optimization
 - Back to hard-margin SVM
 - Soft-margin SVM
 - Large-margin classifiers
- 3 Learning with kernels
 - Kernel methods
 - Positive definite kernels and RKHS
 - Kernel examples
 - Multiple Kernel Learning (MKL)
- 4 Conclusion

Remember: polynomial kernel



$$\forall x, x' \in \mathbb{R}^p, \quad K(x, x') = (x^\top x' + 1)^d$$

is an inner product in a feature space of all monomials of degree up to d

Which functions $K(x, x')$ are kernels?

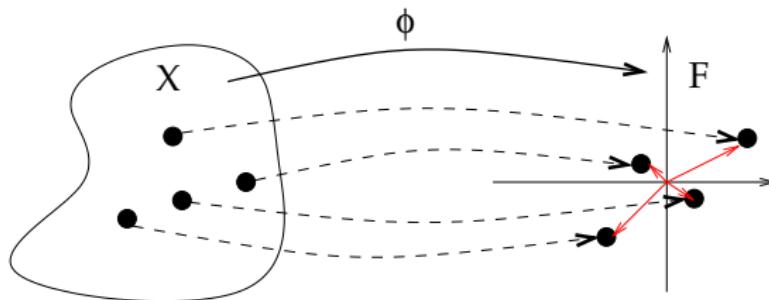
Definition

A function $K(x, x')$ defined on a set \mathcal{X} is a **kernel** if and only if there exists a features space (Hilbert space) \mathcal{H} and a mapping

$$\Phi : \mathcal{X} \mapsto \mathcal{H},$$

such that, for any x, x' in \mathcal{X} :

$$K(x, x') = \langle \Phi(x), \Phi(x') \rangle_{\mathcal{H}}.$$



Reminder ...

- An **inner product** on an \mathbb{R} -vector space \mathcal{H} is a mapping $(f, g) \mapsto \langle f, g \rangle_{\mathcal{H}}$ from \mathcal{H}^2 to \mathbb{R} that is **bilinear, symmetric** and such that $\langle f, f \rangle > 0$ for all $f \in \mathcal{H} \setminus \{0\}$.
- A vector space endowed with an inner product is called **pre-Hilbert**. It is endowed with a norm defined by the inner product as $\|f\|_{\mathcal{H}} = \langle f, f \rangle_{\mathcal{H}}^{\frac{1}{2}}$.
- A **Hilbert space** is a pre-Hilbert space **complete** for the norm defined by the inner product.

Kernel examples

- **Polynomial** (on \mathbb{R}^d):

$$K(x, x') = (x \cdot x' + 1)^d$$

- **Gaussian radial basis function (RBF)** (on \mathbb{R}^d)

$$K(x, x') = \exp\left(-\frac{\|x - x'\|^2}{2\sigma^2}\right)$$

- **Laplace kernel** (on \mathbb{R})

$$K(x, x') = \exp(-\gamma|x - x'|)$$

- **Min kernel** (on \mathbb{R}_+)

$$K(x, x') = \min(x, x')$$

Example: SVM with a Gaussian kernel

- Training:

$$\min_{\alpha \in \mathbb{R}^n} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n \alpha_i \alpha_j y_i y_j \exp\left(-\frac{\|\vec{x}_i - \vec{x}_j\|^2}{2\sigma^2}\right)$$

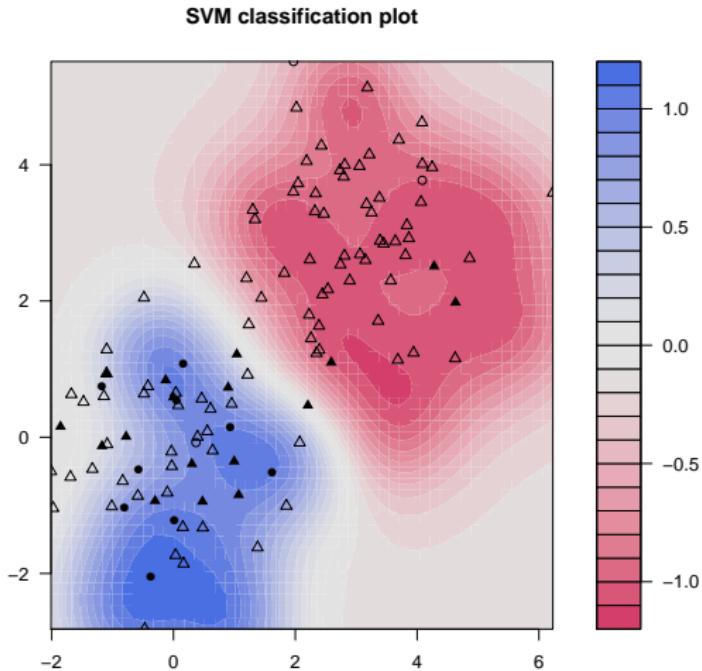
s.t. $0 \leq \alpha_i \leq C$, and $\sum_{i=1}^n \alpha_i y_i = 0$.

- Prediction

$$f(\vec{x}) = \sum_{i=1}^n \alpha_i \exp\left(-\frac{\|\vec{x} - \vec{x}_i\|^2}{2\sigma^2}\right)$$

Example: SVM with a Gaussian kernel

$$f(\vec{x}) = \sum_{i=1}^n \alpha_i \exp\left(-\frac{\|\vec{x} - \vec{x}_i\|^2}{2\sigma^2}\right)$$



Positive Definite (p.d.) functions

Definition

A **positive definite (p.d.) function** on the set \mathcal{X} is a function $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ **symmetric**:

$$\forall (x, x') \in \mathcal{X}^2, \quad K(x, x') = K(x', x),$$

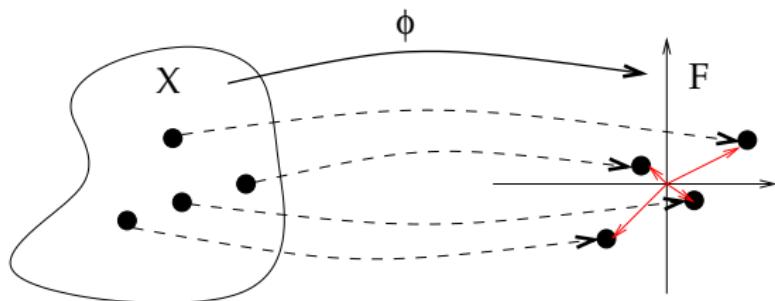
and which satisfies, for all $N \in \mathbb{N}$, $(x_1, x_2, \dots, x_N) \in \mathcal{X}^N$ et $(a_1, a_2, \dots, a_N) \in \mathbb{R}^N$:

$$\sum_{i=1}^N \sum_{j=1}^N a_i a_j K(x_i, x_j) \geq 0.$$

Kernels are p.d. functions

Theorem (Aronszajn, 1950)

K is a kernel if and only if it is a positive definite function.



Proof: kernel \implies p.d. (easy)

Let

$$K(x, x') = \langle \Phi(x), \Phi(x') \rangle_{\mathcal{H}}$$

be a kernel. It is p.d. because:

- $K(x, x') = \langle \Phi(x), \Phi(x') \rangle_{\mathcal{H}} = \langle \Phi(x'), \Phi(x) \rangle_{\mathcal{H}} = K(x', x)$,
- $\sum_{i=1}^N \sum_{j=1}^N a_i a_j \langle \Phi(x_i), \Phi(x_j) \rangle_{\mathcal{H}} = \| \sum_{i=1}^N a_i \Phi(x_i) \|_{\mathcal{H}}^2 \geq 0$.

Proof: p.d. \implies kernel when \mathcal{X} is finite

- Suppose $\mathcal{X} = \{x_1, x_2, \dots, x_N\}$ is finite of size N .
- Any p.d. kernel $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is entirely defined by the $N \times N$ symmetric positive semidefinite matrix $[K]_{ij} := K(x_i, x_j)$.
- It can therefore be diagonalized on an orthonormal basis of eigenvectors (u_1, u_2, \dots, u_N) , with non-negative eigenvalues $0 \leq \lambda_1 \leq \dots \leq \lambda_N$, i.e.,

$$K(x_i, x_j) = \left[\sum_{l=1}^N \lambda_l u_l u_l^\top \right]_{ij} = \sum_{l=1}^N \lambda_l u_l(i) u_l(j) = \langle \Phi(x_i), \Phi(x_j) \rangle_{\mathbb{R}^N},$$

with

$$\Phi(x_i) = \begin{pmatrix} \sqrt{\lambda_1} u_1(i) \\ \vdots \\ \sqrt{\lambda_N} u_N(i) \end{pmatrix}. \quad \square$$

Proof: p.d. \implies kernel in the general case

- Mercer (1909) for $\mathcal{X} = [a, b] \subset \mathbb{R}$ (more generally \mathcal{X} compact) and K continuous (the so-called **Mercer kernels**).
- Kolmogorov (1941) for \mathcal{X} countable.
- Aronszajn (1944, 1950) for the general case, using the theory of RKHS.

Definition

Let \mathcal{X} be a set and $\mathcal{H} \subset \mathbb{R}^{\mathcal{X}}$ be a class of functions forming a (real) Hilbert space with inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$. The function $K : \mathcal{X}^2 \mapsto \mathbb{R}$ is called a reproducing kernel (r.k.) of \mathcal{H} if

- ① \mathcal{H} contains all functions of the form

$$\forall x \in \mathcal{X}, \quad K_x : t \mapsto K(x, t).$$

- ② For every $x \in \mathcal{X}$ and $f \in \mathcal{H}$ the reproducing property holds:

$$f(x) = \langle f, K_x \rangle_{\mathcal{H}}.$$

If a r.k. exists, then \mathcal{H} is called a reproducing kernel Hilbert space (RKHS).

An equivalent definition of RKHS

Theorem

The Hilbert space $\mathcal{H} \subset \mathbb{R}^{\mathcal{X}}$ is a RKHS if and only if for any $x \in \mathcal{X}$, the mapping:

$$\begin{aligned} F : \quad & \mathcal{H} \rightarrow \mathbb{R} \\ f & \mapsto f(x) \end{aligned}$$

is **continuous**.

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is **continuous**.

Corollary

Convergence in a RKHS implies pointwise convergence, i.e., if $(f_n)_{n \in \mathbb{N}}$ converges to f in \mathcal{H} , then $(f_n(x))_{n \in \mathbb{N}}$ converges to $f(x)$ for any $x \in \mathcal{X}$.

Proof

If \mathcal{H} is a RKHS then $f \mapsto f(x)$ is continuous

If a r.k. K exists, then for any $(x, f) \in \mathcal{X} \times \mathcal{H}$:

$$\begin{aligned}|f(x)| &= |\langle f, K_x \rangle_{\mathcal{H}}| \\&\leq \|f\|_{\mathcal{H}} \cdot \|K_x\|_{\mathcal{H}} \text{ (Cauchy-Schwarz)} \\&\leq \|f\|_{\mathcal{H}} \cdot K(x, x)^{\frac{1}{2}},\end{aligned}$$

because $\|K_x\|_{\mathcal{H}}^2 = \langle K_x, K_x \rangle_{\mathcal{H}} = K(x, x)$. Therefore $f \in \mathcal{H} \mapsto f(x) \in \mathbb{R}$ is a continuous linear mapping. \square

Proof (Converse)

If $f \mapsto f(x)$ is continuous then \mathcal{H} is a RKHS

Conversely, let us assume that for any $x \in \mathcal{X}$ the linear form $f \in \mathcal{H} \mapsto f(x)$ is continuous.

Then by Riesz representation theorem there (general property of Hilbert spaces) there exists a unique $g_x \in \mathcal{H}$ such that:

$$f(x) = \langle f, g_x \rangle_{\mathcal{H}}$$

The function $K(x, y) = g_x(y)$ is then a r.k. for \mathcal{H} . \square

Unicity of r.k. and RKHS

Theorem

- If \mathcal{H} is a RKHS, then it has a unique r.k.
- Conversely, a function K can be the r.k. of at most one RKHS.

Unicity of r.k. and RKHS

Theorem

- If \mathcal{H} is a RKHS, then it has a unique r.k.
- Conversely, a function K can be the r.k. of at most one RKHS.

Consequence

This shows that we can talk of "the" kernel of a RKHS, or "the" RKHS of a kernel.

Proof

If a r.k. exists then it is unique

Let K and K' be two r.k. of a RKHS \mathcal{H} . Then for any $x \in \mathcal{X}$:

$$\begin{aligned}\|K_x - K'_x\|_{\mathcal{H}}^2 &= \langle K_x - K'_x, K_x - K'_x \rangle_{\mathcal{H}} \\&= \langle K_x - K'_x, K_x \rangle_{\mathcal{H}} - \langle K_x - K'_x, K'_x \rangle_{\mathcal{H}} \\&= K_x(x) - K'_x(x) - K_x(x) + K'_x(x) \\&= 0.\end{aligned}$$

This shows that $K_x = K'_x$ as functions, i.e., $K_x(y) = K'_x(y)$ for any $y \in \mathcal{X}$.
In other words, $\mathbf{K}=\mathbf{K}'$. \square

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The RKHS of a r.k. K is unique

Left as exercise.

An important result

Theorem

A function $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is p.d. if and only if it is a r.k.

Proof: r.k. \implies p.d.

- ① A r.k. is **symmetric** because, for any $(x, y) \in \mathcal{X}^2$:

$$K(x, y) = \langle K_x, K_y \rangle_{\mathcal{H}} = \langle K_y, K_x \rangle_{\mathcal{H}} = K(y, x).$$

- ② It is **p.d.** because for any $N \in \mathbb{N}, (x_1, x_2, \dots, x_N) \in \mathcal{X}^N$, and $(a_1, a_2, \dots, a_N) \in \mathbb{R}^N$:

$$\begin{aligned} \sum_{i,j=1}^N a_i a_j K(x_i, x_j) &= \sum_{i,j=1}^N a_i a_j \langle K_{x_i}, K_{x_j} \rangle_{\mathcal{H}} \\ &= \| \sum_{i=1}^N a_i K_{x_i} \|_{\mathcal{H}}^2 \\ &\geq 0. \quad \square \end{aligned}$$

Proof: p.d. \implies r.k. (1/4)

- Let \mathcal{H}_0 be the vector subspace of $\mathbb{R}^{\mathcal{X}}$ spanned by the functions $\{K_x\}_{x \in \mathcal{X}}$.
- For any $f, g \in \mathcal{H}_0$, given by:

$$f = \sum_{i=1}^m a_i K_{x_i}, \quad g = \sum_{j=1}^n b_j K_{y_j},$$

let:

$$\langle f, g \rangle_{\mathcal{H}_0} := \sum_{i,j} a_i b_j K(x_i, y_j).$$

Proof: p.d. \implies r.k. (2/4)

- $\langle f, g \rangle_{\mathcal{H}_0}$ does not depend on the expansion of f and g because:

$$\langle f, g \rangle_{\mathcal{H}_0} = \sum_{i=1}^m a_i g(x_i) = \sum_{j=1}^n b_j f(y_j).$$

- This also shows that $\langle \cdot, \cdot \rangle_{\mathcal{H}_0}$ is a symmetric bilinear form.
- This also shows that for any $x \in \mathcal{X}$ and $f \in \mathcal{H}_0$:

$$\langle f, K_x \rangle_{\mathcal{H}_0} = f(x).$$

Proof: p.d. \implies r.k. (3/4)

- K is assumed to be p.d., therefore:

$$\|f\|_{\mathcal{H}_0}^2 = \sum_{i,j=1}^m a_i a_j K(x_i, x_j) \geq 0.$$

In particular Cauchy-Schwarz is valid with $\langle \cdot, \cdot \rangle_{\mathcal{H}_0}$.

- By Cauchy-Schwarz we deduce that $\forall x \in \mathcal{X}$:

$$|f(x)| = |\langle f, K_x \rangle_{\mathcal{H}_0}| \leq \|f\|_{\mathcal{H}_0} \cdot K(x, x)^{\frac{1}{2}},$$

therefore $\|f\|_{\mathcal{H}_0} = 0 \implies f = 0$.

- \mathcal{H}_0 is therefore a **pre-Hilbert space** endowed with the inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}_0}$.

Proof: p.d. \implies r.k. (4/4)

- For any Cauchy sequence $(f_n)_{n \geq 0}$ in $(\mathcal{H}_0, \langle \cdot, \cdot \rangle_{\mathcal{H}_0})$, we note that:

$$\forall (x, m, n) \in \mathcal{X} \times \mathbb{N}^2, \quad |f_m(x) - f_n(x)| \leq \|f_m - f_n\|_{\mathcal{H}_0} K(x, x)^{\frac{1}{2}}.$$

Therefore for any x the sequence $(f_n(x))_{n \geq 0}$ is Cauchy in \mathbb{R} and has therefore a limit.

- If we add to \mathcal{H}_0 the functions defined as the pointwise limits of Cauchy sequences, then the space becomes complete and is therefore a Hilbert space, with K as r.k. (up to a few technicalities, left as exercice). \square

Application: back to Aronszajn's theorem

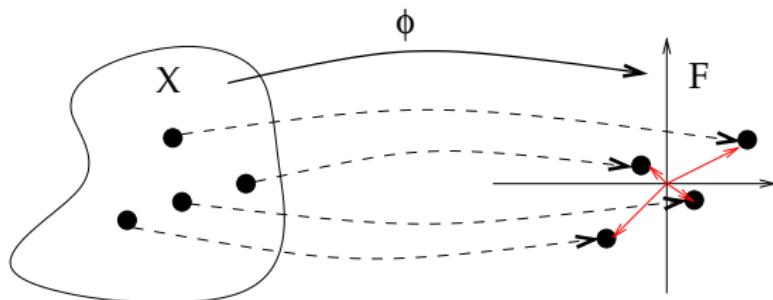
Theorem (Aronszajn, 1950)

K is a p.d. kernel on the set \mathcal{X} if and only if there exists a Hilbert space \mathcal{H} and a mapping

$$\Phi : \mathcal{X} \mapsto \mathcal{H},$$

such that, for any x, x' in \mathcal{X} :

$$K(x, x') = \langle \Phi(x), \Phi(x') \rangle_{\mathcal{H}}.$$



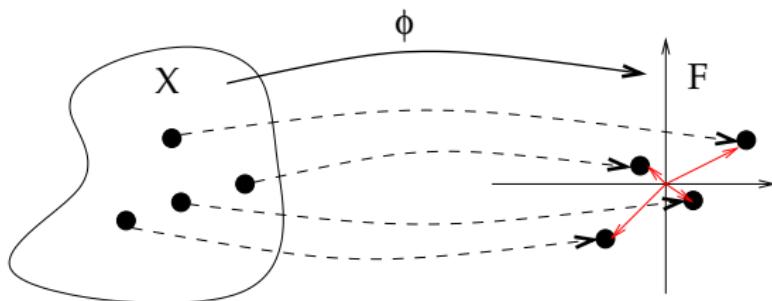
Proof of Aronzsajn's theorem: p.d. \implies kernel

- If K is p.d. over a set \mathcal{X} then it is the r.k. of a Hilbert space $\mathcal{H} \subset \mathbb{R}^{\mathcal{X}}$.
- Let the mapping $\Phi : \mathcal{X} \rightarrow \mathcal{H}$ defined by:

$$\forall x \in \mathcal{X}, \quad \Phi(x) = K_x.$$

- By the reproducing property we have:

$$\forall (x, y) \in \mathcal{X}^2, \quad \langle \Phi(x), \Phi(y) \rangle_{\mathcal{H}} = \langle K_x, K_y \rangle_{\mathcal{H}} = K(x, y). \quad \square$$



RKHS of the linear kernel

- Let $\mathcal{X} = \mathbb{R}^d$ and $K(x, y) = \langle x, y \rangle_{\mathbb{R}^d}$ be the linear kernel
- The corresponding RKHS consists of functions:

$$x \in \mathbb{R}^d \mapsto f(x) = \sum_i a_i \langle x_i, x \rangle_{\mathbb{R}^d} = \langle w, x \rangle_{\mathbb{R}^d},$$

with $w = \sum_i a_i x_i$.

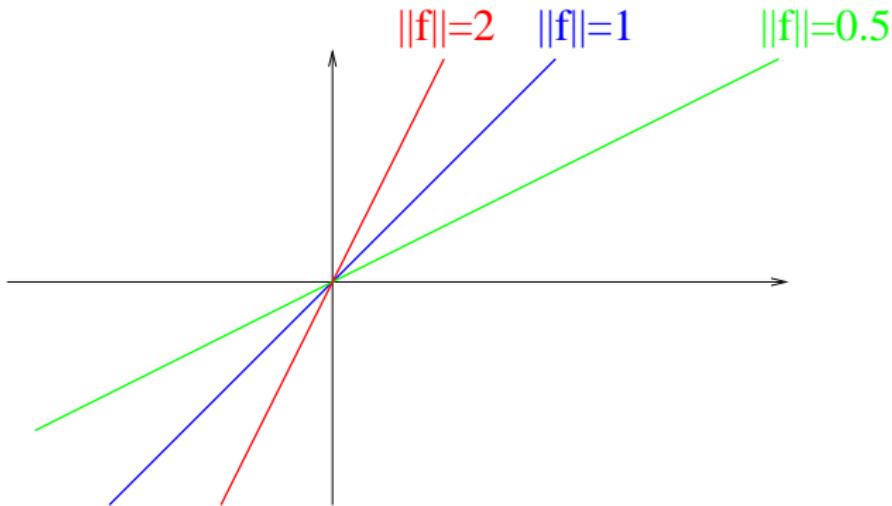
- The RKHS is therefore the set of linear forms endowed with the following inner product:

$$\langle f, g \rangle_{\mathcal{H}_K} = \langle w, v \rangle_{\mathbb{R}^d},$$

when $f(x) = w^\top x$ and $g(x) = v^\top x$.

RKHS of the linear kernel (cont.)

$$\begin{cases} K_{lin}(x, x') &= x^\top x' \\ f(x) &= w^\top x, \\ \|f\|_{\mathcal{H}} &= \|w\|_2. \end{cases}$$



ℓ_2 -regularized methods in RKHS

$$f_\beta(x) = \beta^\top \Phi(x), \quad \min_{\beta \in \mathbb{R}^p} \left\{ \frac{1}{n} \sum_{i=1}^n \ell(f_\beta(x_i), y_i) + \lambda \|\beta\|_2^2 \right\}$$

is equivalent to

$$\min_{f \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{i=1}^n \ell(f(x_i), y_i) + \lambda \|f\|_{\mathcal{H}}^2 \right\}$$

where \mathcal{H} is the RKHS of the kernel $K(x, x') = \Phi(x)^\top \Phi(x')$.

Smoothness functional

A simple inequality

- By Cauchy-Schwarz we have, for any function $f \in \mathcal{H}$ and any two points $x, x' \in \mathcal{X}$:

$$\begin{aligned} |f(x) - f(x')| &= |\langle f, K_x - K_{x'} \rangle_{\mathcal{H}}| \\ &\leq \|f\|_{\mathcal{H}} \times \|K_x - K_{x'}\|_{\mathcal{H}} \\ &= \|f\|_{\mathcal{H}} \times d_K(x, x'). \end{aligned}$$

- The norm of a function in the RKHS controls **how fast** the function varies over \mathcal{X} with respect to the **geometry defined by the kernel** (Lipschitz with constant $\|f\|_{\mathcal{H}}$).

Important message

Small norm \implies slow variations.

Kernels and RKHS : Summary

- P.d. kernels can be thought of as **inner product** after embedding the data space \mathcal{X} in some Hilbert space. As such a p.d. kernel defines a **metric** on \mathcal{X} .
- A realization of this embedding is the **RKHS**, valid without restriction on the space \mathcal{X} nor on the kernel.
- The RKHS is a space of functions over \mathcal{X} . The **norm** of a function in the RKHS is related to its degree of **smoothness** w.r.t. the metric defined by the kernel on \mathcal{X} .
- ℓ_2 -regularized learning in the feature space can be formulated in the RKHS

$$\min_{f \in \mathcal{H}} \left\{ \frac{1}{n} \sum_{i=1}^n \ell(f(x_i), y_i) + \lambda \|f\|_{\mathcal{H}}^2 \right\}$$

Outline

- 1 Learning in high dimension
- 2 Learning with ℓ_2 regularization
 - Ridge regression
 - Ridge logistic regression
 - Linear hard-margin SVM
 - Interlude: quick notes on constrained optimization
 - Back to hard-margin SVM
 - Soft-margin SVM
 - Large-margin classifiers
- 3 Learning with kernels
 - Kernel methods
 - Positive definite kernels and RKHS
 - **Kernel examples**
 - Multiple Kernel Learning (MKL)
- 4 Conclusion

Kernel examples

- **Polynomial** (on \mathbb{R}^d):

$$K(x, x') = (x \cdot x' + 1)^d$$

- **Gaussian radial basis function (RBF)** (on \mathbb{R}^d)

$$K(x, x') = \exp\left(-\frac{\|x - x'\|^2}{2\sigma^2}\right)$$

- **Laplace kernel** (on \mathbb{R})

$$K(x, x') = \exp(-\gamma|x - x'|)$$

- **Min kernel** (on \mathbb{R}_+)

$$K(x, x') = \min(x, x')$$

Exercice

Exercice: for each kernel, find a Hilbert space \mathcal{H} and a mapping $\Phi : \mathcal{X} \rightarrow \mathcal{H}$ such that $K(x, x') = \langle \Phi(x), \Phi(x') \rangle$

Example: SVM with a Gaussian kernel

- Training:

$$\min_{\alpha \in \mathbb{R}^n} \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n \alpha_i \alpha_j y_i y_j \exp\left(-\frac{\|\vec{x}_i - \vec{x}_j\|^2}{2\sigma^2}\right)$$

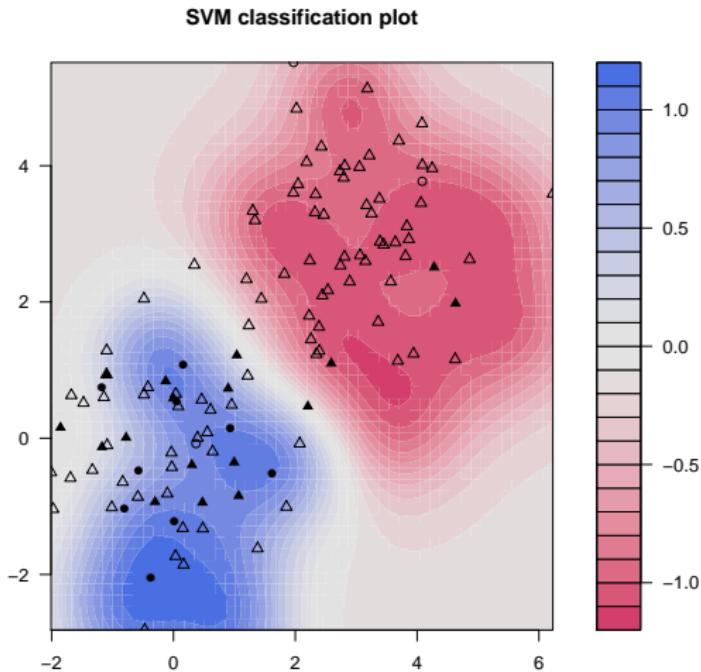
$$\text{s.t. } 0 \leq \alpha_i \leq C, \quad \text{and} \quad \sum_{i=1}^n \alpha_i y_i = 0.$$

- Prediction

$$f(\vec{x}) = \sum_{i=1}^n \alpha_i \exp\left(-\frac{\|\vec{x} - \vec{x}_i\|^2}{2\sigma^2}\right)$$

Example: SVM with a Gaussian kernel

$$f(\vec{x}) = \sum_{i=1}^n \alpha_i \exp\left(-\frac{\|\vec{x} - \vec{x}_i\|^2}{2\sigma^2}\right)$$



How to choose or make a kernel?

- Design **features**
- Design a **distance** or **similarity** measure
- Design a **regularizer** on f

Example: Sobolev norm as regularizer

Theorem

Let $\mathcal{X} = [0, 1]$ and the kernel:

$$\forall (x, y) \in [0, 1]^2, \quad K(x, y) = \min(x, y).$$

Then the RKHS is

$$\mathcal{H} = \{f : [0, 1] \mapsto \mathbb{R}, \text{absolutely continuous, } f' \in L^2([0, 1]), f(0) = 0\}.$$

and the regularizer is a Sobolev norm

$$\Omega(f) = \|f\|_{\mathcal{H}}^2 = \int_0^1 f'(u)^2 du = \|f'\|_{L^2([0,1])}^2.$$

Proof (1/5)

Sketch

We need to show that

- \mathcal{H} is a Hilbert space
- $\forall x \in [0, 1], K_x \in \mathcal{H},$
- $\forall (x, f) \in [0, 1] \times \mathcal{H}, \langle f, K_x \rangle_{\mathcal{H}} = f(x).$

Proof (2/5)

\mathcal{H} is a pre-Hilbert space

- f absolutely continuous implies differentiable almost everywhere, and

$$\forall x \in [0, 1], \quad f(x) = f(0) + \int_0^x f'(u)du.$$

- For any $f \in \mathcal{H}$, $f(0) = 0$ implies by Cauchy-Schwarz:

$$|f(x)| = \left| \int_0^x f'(u)du \right| \leq \sqrt{x} \left(\int_0^1 f'(u)^2 du \right)^{\frac{1}{2}} = \sqrt{x} \|f\|_{\mathcal{H}}.$$

Therefore, $\|f\|_{\mathcal{H}} = 0 \implies f = 0$, showing that $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ is an inner product. \mathcal{H} is thus a pre-Hilbert space.

Proof (3/5)

\mathcal{H} is a Hilbert space

- To show that \mathcal{H} is complete, let $(f_n)_{n \in \mathbb{N}}$ a Cauchy sequence in \mathcal{H}
- $(f'_n)_{n \in \mathbb{N}}$ is a Cauchy sequence in $L^2[0, 1]$, thus converges to $g \in L^2[0, 1]$
- By the previous inequality, $(f_n(x))_{n \in \mathbb{N}}$ is a Cauchy sequence and thus converges to a real number $f(x)$, for any $x \in [0, 1]$. Moreover:

$$f(x) = \lim_n f_n(x) = \lim_n \int_0^x f'_n(u) du = \int_0^x g(u) du,$$

showing that f is absolutely continuous and $f' = g$ almost everywhere; in particular, $f' \in L^2[0, 1]$.

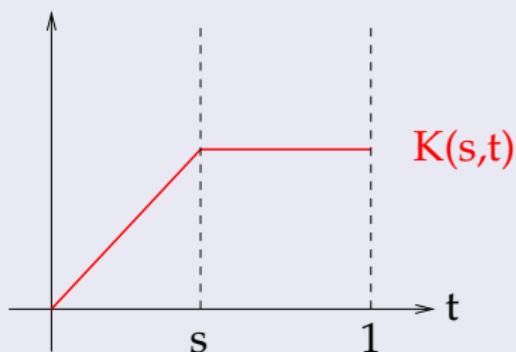
- Finally, $f(0) = \lim_n f_n(0) = 0$, therefore $f \in \mathcal{H}$ and

$$\lim_n \|f_n - f\|_{\mathcal{H}} = \|f' - g\|_{L^2[0,1]} = 0.$$

Proof (4/5)

$\forall x \in [0, 1], K_x \in \mathcal{H}$

Let $K_x(y) = K(x, y) = \min(x, y)$ sur $[0, 1]^2$:



K_x is differentiable except at s , has a square integrable derivative, and $K_x(0) = 0$, therefore $K_x \in \mathcal{H}$ for all $x \in [0, 1]$. \square

Proof (5/5)

For all x, f , $\langle f, K_x \rangle_{\mathcal{H}} = f(x)$

For any $x \in [0, 1]$ and $f \in \mathcal{H}$ we have:

$$\langle f, K_x \rangle_{\mathcal{H}} = \int_0^1 f'(u) K'_x(u) du = \int_0^x f'(u) du = f(x),$$

which shows that K is the r.k. associated to \mathcal{H} . \square

Generalization

Theorem

Let $\mathcal{X} = \mathbb{R}^d$ and D a differential operator on a class of functions \mathcal{H} such that, endowed with the inner product:

$$\forall (f, g) \in \mathcal{H}^2, \quad \langle f, g \rangle_{\mathcal{H}} = \langle Df, Dg \rangle_{L^2(\mathcal{X})},$$

it is a Hilbert space.

Then \mathcal{H} is a RKHS that admits as r.k. the Green function of the operator D^*D , where D^* denotes the adjoint operator of D .

In case of...

Green functions

Let the differential equation on \mathcal{H} :

$$f = Dg ,$$

where g is unknown. In order to solve it we can look for g of the form:

$$g(x) = \int_{\mathcal{X}} k(x, y) f(y) dy$$

for some function $k : \mathcal{X}^2 \mapsto \mathbb{R}$. k must then satisfy, for all $x \in \mathcal{X}$,

$$f(x) = Dg(x) = \langle Dk_x, f \rangle_{L^2(\mathcal{X})} .$$

k is called the **Green function** of the operator D .

Proof

Let \mathcal{H} be a Hilbert space endowed with the inner product:

$$\langle f, g \rangle_{\mathcal{X}} = \langle Df, Dg \rangle_{L^2(\mathcal{X})},$$

and K be the Green function of the operator D^*D . For all $x \in \mathcal{X}$, $K_x \in \mathcal{H}$ because:

$$\langle DK_x, DK_x \rangle_{L^2(\mathcal{X})} = \langle D^*DK_x, K_x \rangle_{L^2(\mathcal{X})} = K_x(x) < \infty.$$

Moreover, for all $f \in \mathcal{H}$ and $x \in \mathcal{X}$, we have:

$$f(x) = \langle D^*DK_x, f \rangle_{L^2(\mathcal{X})} = \langle DK_x, Df \rangle_{L^2(\mathcal{X})} = \langle K_x, f \rangle_{\mathcal{H}},$$

which shows that \mathcal{H} is a RKHS with K as r.k. \square

Translation invariant kernels

Definition

A kernel $K : \mathbb{R}^d \times \mathbb{R}^d \mapsto \mathbb{R}$ is called **translation invariant** (t.i.) if it only depends on the difference between its arguments, i.e.:

$$\forall (x, y) \in \mathbb{R}^{2d}, \quad K(x, y) = \kappa(x - y).$$

Theorem (Bochner)

A real-valued function $\kappa(x - y)$ on \mathbb{R}^d is positive definite if and only if it is the Fourier transform of a **symmetric, positive, and finite** Borel measure.

RKHS of translation invariant kernels

Theorem

Let K be a translation invariant p.d. kernel, such that κ is integrable on \mathbb{R}^d as well as its Fourier transform $\hat{\kappa}$. The subset \mathcal{H}_K of $L_2(\mathbb{R}^d)$ that consists of integrable and continuous functions f such that:

$$\|f\|_K^2 := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{|\hat{f}(\omega)|^2}{\hat{\kappa}(\omega)} d\omega < +\infty,$$

endowed with the inner product:

$$\langle f, g \rangle := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{\hat{f}(\omega) \hat{g}(\omega)^*}{\hat{\kappa}(\omega)} d\omega$$

is a RKHS with K as r.k.

Example: Gaussian RBF kernel

$$K(x, y) = e^{-\frac{(x-y)^2}{2\sigma^2}}$$

corresponds to:

$$\hat{\kappa}(\omega) = e^{-\frac{\sigma^2 \omega^2}{2}}$$

and

$$\|f\|_{\mathcal{H}}^2 = \int \left| \hat{f}(\omega) \right|^2 e^{\frac{\sigma^2 \omega^2}{2}} d\omega.$$

In particular, all functions in \mathcal{H} are **infinitely differentiable** with all derivatives in L^2 .

Example: Laplace kernel

$$K(x, y) = \frac{1}{2} e^{-\gamma|x-y|}$$

corresponds to:

$$\hat{\kappa}(\omega) = \frac{\gamma}{\gamma^2 + \omega^2}$$

and

$$\|f\|_{\mathcal{H}}^2 = \int \left| \hat{f}(\omega) \right|^2 \frac{(\gamma^2 + \omega^2)}{\gamma} d\omega.$$

The RKHS is the set of functions L^2 differentiable with derivatives in L^2 (Sobolev space).

Example: sinc kernel

$$K(x, y) = \frac{\sin(\Omega(x - y))}{\pi(x - y)}$$

corresponds to:

$$\hat{\kappa}(\omega) = \mathbf{1}(-\Omega \leq \omega \leq \Omega).$$

The RKHS is the set of functions whose spectrum is included in $[-\Omega, \Omega]$:

$$\mathcal{H} = \left\{ f : \int_{|\omega| > \Omega} |\hat{f}(\omega)|^2 d\omega = 0 \right\},$$

and

$$\|f\|_{\mathcal{H}}^2 = \int_{|\omega| \leq \Omega} |\hat{f}(\omega)|^2 = \int_{\omega \in \mathbb{R}} |\hat{f}(\omega)|^2 = (2\pi)^d \int_{x \in \mathbb{R}} |f(x)|^2 dx.$$

Supervised sequence classification

Data (training)

- Secreted proteins:

MASKATLLLAFATLLFATCIARHQQRQQQNQCQLQNIEA...

MARSSLFTFLCLAVFINGCLSQIEQQSPWEFQGSEVW...

MALHTVLIMLSLLPMLEAQNPEHANITIGEPITNETLGWL...

...

- Non-secreted proteins:

MAPPSSVFAEVPQAQPVLVFKLIADFREDPDPRKVN LGVG...

MAHTLGLTQPNSTEPHKISFTAKEIDVIEWKG DILVVG...

MSISESYAKEIKTAFRQFTDFPIEGEQFEDFLPIIGNP..

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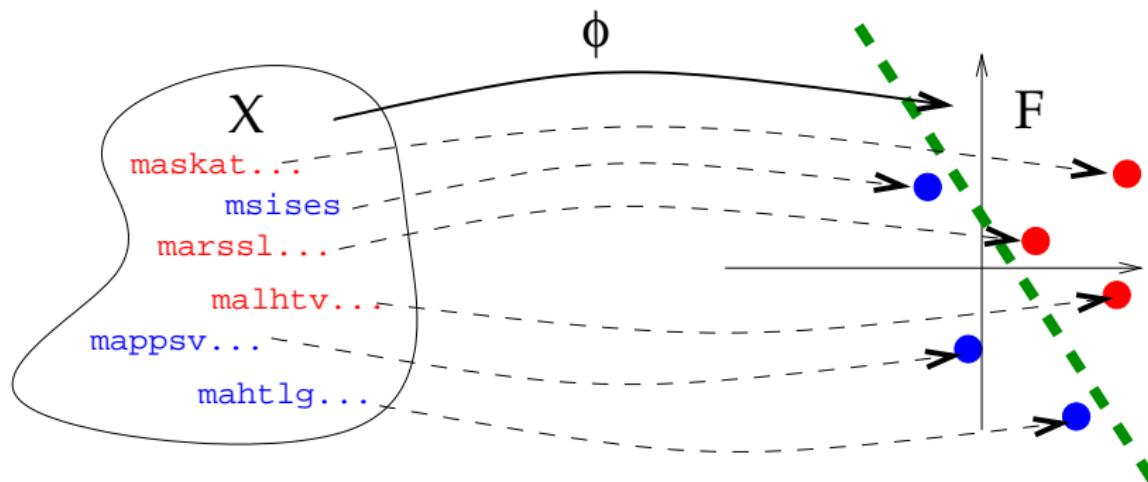
Goal

- Build a **classifier** to **predict** whether new proteins are secreted or not.

String kernels

The idea

- Map each string $x \in \mathcal{X}$ to a vector $\Phi(x) \in \mathcal{F}$.
- Train a **classifier for vectors** on the images $\Phi(x_1), \dots, \Phi(x_n)$ of the training set (nearest neighbor, linear perceptron, logistic regression, support vector machine...)



Example: substring indexation

The approach

Index the feature space by fixed-length strings, i.e.,

$$\Phi(x) = (\Phi_u(x))_{u \in \mathcal{A}^k}$$

where $\Phi_u(x)$ can be:

- the number of occurrences of u in x (without gaps) : **spectrum kernel** (Leslie et al., 2002)
- the number of occurrences of u in x up to m mismatches (without gaps) : **mismatch kernel** (Leslie et al., 2004)
- the number of occurrences of u in x allowing gaps, with a weight decaying exponentially with the number of gaps : **substring kernel** (Lohdi et al., 2002)

Spectrum kernel (1/2)

Kernel definition

- The 3-spectrum of

$$x = \text{CGGSLIAMMWFGV}$$

is:

$(\text{CGG}, \text{GGS}, \text{GSL}, \text{SLI}, \text{LIA}, \text{IAM}, \text{AMM}, \text{MMW}, \text{MWF}, \text{WFG}, \text{FGV})$.

- Let $\Phi_u(x)$ denote the number of occurrences of u in x . The k -spectrum kernel is:

$$K(x, x') := \sum_{u \in \mathcal{A}^k} \Phi_u(x) \Phi_u(x')$$

Spectrum kernel (2/2)

Implementation

- The computation of the kernel is formally a sum over $|\mathcal{A}|^k$ terms, but at most $|x| - k + 1$ terms are non-zero in $\Phi(x) \implies$ Computation in $O(|x| + |x'|)$ with pre-indexation of the strings.
- Fast classification of a sequence x in $O(|x|)$:

$$f(x) = w \cdot \Phi(x) = \sum_u w_u \Phi_u(x) = \sum_{i=1}^{|x|-k+1} w_{x_i \dots x_{i+k-1}}.$$

Remarks

- Work with any string (natural language, time series...)
- Fast and scalable, a good default method for string classification.
- Variants allow matching of k -mers up to m mismatches.

Local alignment kernel (Saigo et al., 2004)

CGGSLIAMM-----WFGV
| ... | | | | . . . | | | |
C----LIVMMNRLMWFGV

$$\begin{aligned}s_{S,g}(\pi) &= S(C, C) + S(L, L) + S(I, I) + S(A, V) + 2S(M, M) \\&\quad + S(W, W) + S(F, F) + S(G, G) + S(V, V) - g(3) - g(4)\end{aligned}$$

$$SW_{S,g}(x, y) := \max_{\pi \in \Pi(x, y)} s_{S,g}(\pi) \quad \text{is not a kernel}$$

$$K_{LA}^{(\beta)}(x, y) = \sum_{\pi \in \Pi(x, y)} \exp(\beta s_{S,g}(x, y, \pi)) \quad \text{is a kernel}$$

LA kernel is p.d.: proof (1/2)

Definition: Convolution kernel (Haussler, 1999)

Let K_1 and K_2 be two p.d. kernels for strings. The convolution of K_1 and K_2 , denoted $K_1 \star K_2$, is defined for any $x, x' \in \mathcal{X}$ by:

$$K_1 \star K_2(x, y) := \sum_{x_1 x_2 = x, y_1 y_2 = y} K_1(x_1, y_1) K_2(x_2, y_2).$$

Lemma

If K_1 and K_2 are p.d. then $K_1 \star K_2$ is p.d..

LA kernel is p.d.: proof (2/2)

$$K_{LA}^{(\beta)} = \sum_{n=0}^{\infty} K_0 \star \left(K_a^{(\beta)} \star K_g^{(\beta)} \right)^{(n-1)} \star K_a^{(\beta)} \star K_0 ,$$

with

- The constant kernel:

$$K_0(x, y) := 1 .$$

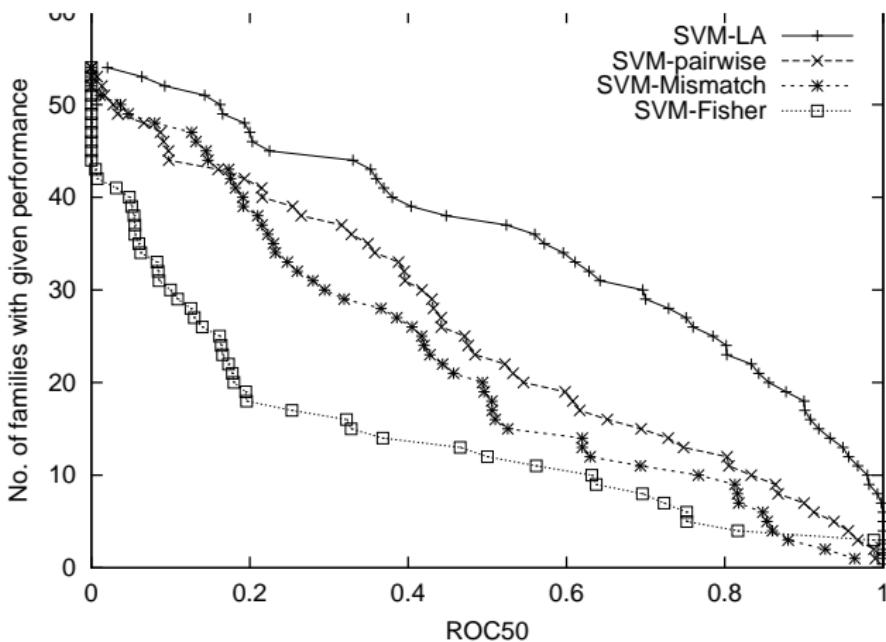
- A kernel for letters:

$$K_a^{(\beta)}(x, y) := \begin{cases} 0 & \text{if } |x| \neq 1 \text{ where } |y| \neq 1 , \\ \exp(\beta S(x, y)) & \text{otherwise .} \end{cases}$$

- A kernel for gaps:

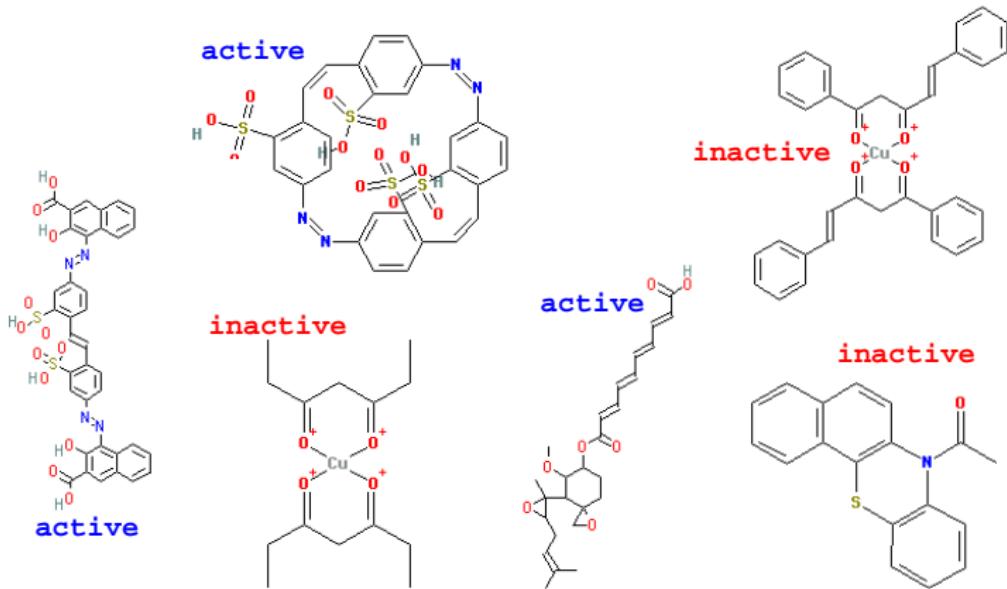
$$K_g^{(\beta)}(x, y) = \exp[\beta(g(|x|) + g(|y|))] .$$

The choice of kernel matters



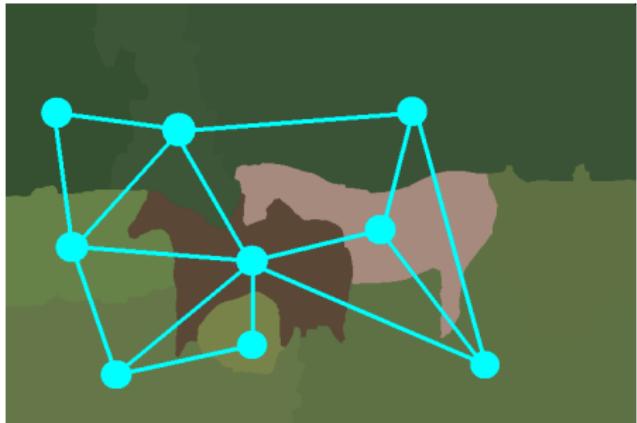
Performance on the SCOP superfamily recognition benchmark (from Saigo et al., 2004).

Virtual screening for drug discovery



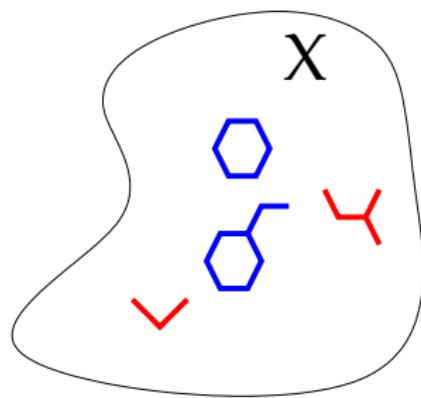
NCI AIDS screen results (from <http://cactus.nci.nih.gov>).

Image retrieval and classification



From Harchaoui and Bach (2007).

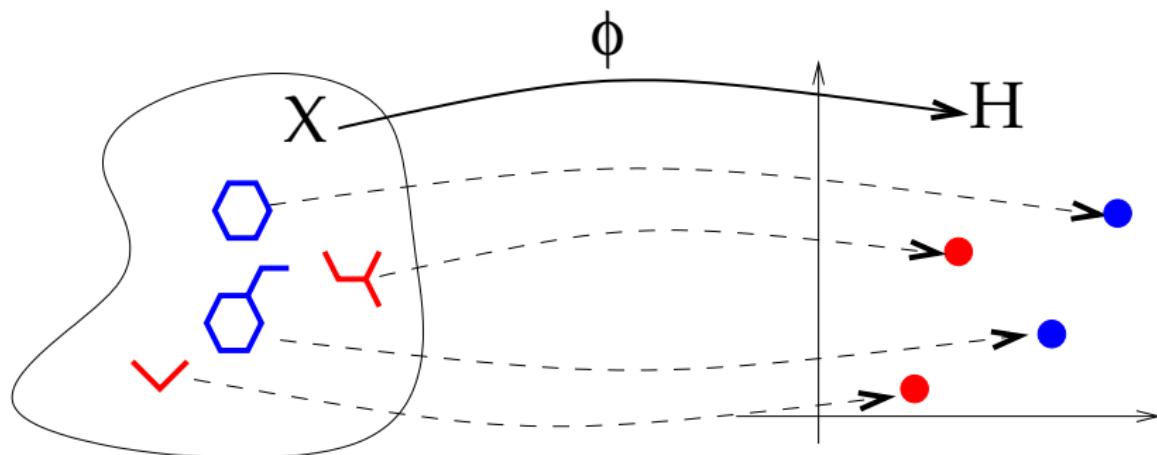
Graph kernels



Graph kernels

- ① Represent each graph x by a vector $\Phi(x) \in \mathcal{H}$, either **explicitly** or **implicitly** through the kernel

$$K(x, x') = \Phi(x)^\top \Phi(x').$$

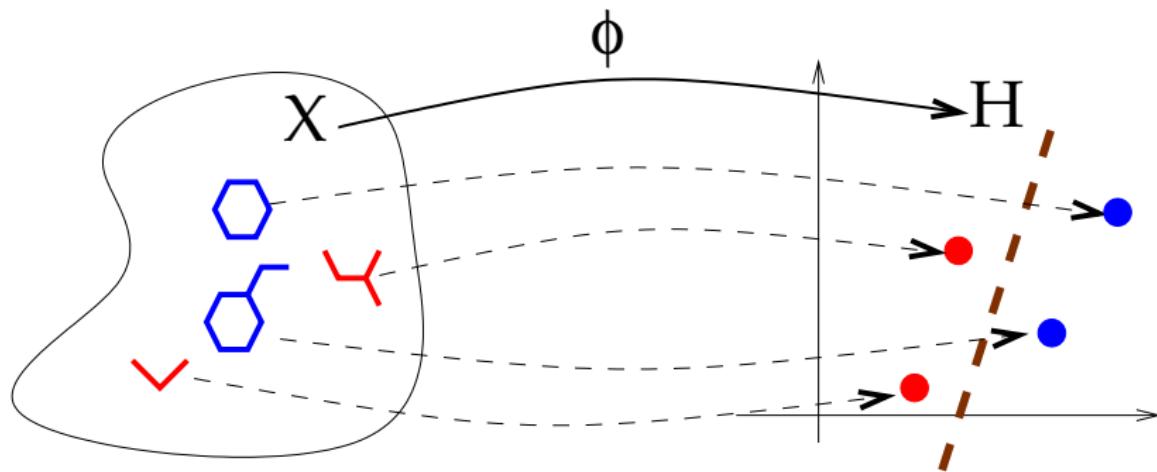


Graph kernels

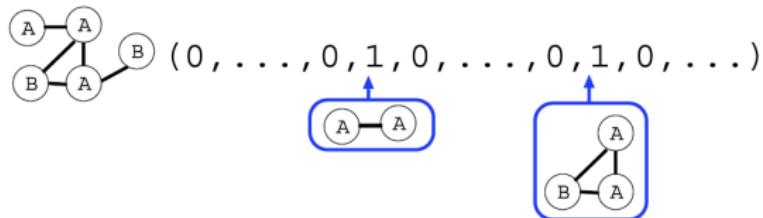
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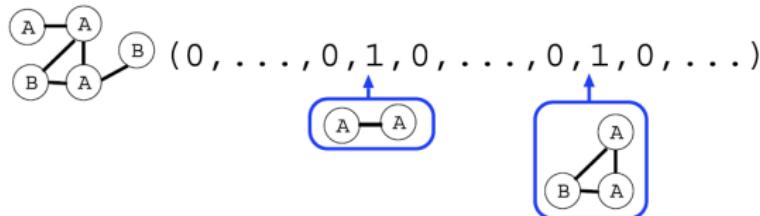
- ② Use a linear method for classification in \mathcal{H} .



Indexing by all subgraphs?



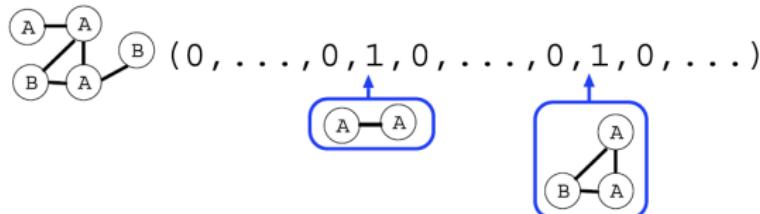
Indexing by all subgraphs?



Theorem

Computing all subgraph occurrences is NP-hard.

Indexing by all subgraphs?



Theorem

Computing all subgraph occurrences is NP-hard.

Proof.

- The linear graph of size n is a subgraph of a graph X with n vertices iff X has an Hamiltonian path
- The decision problem whether a graph has a Hamiltonian path is NP-complete.



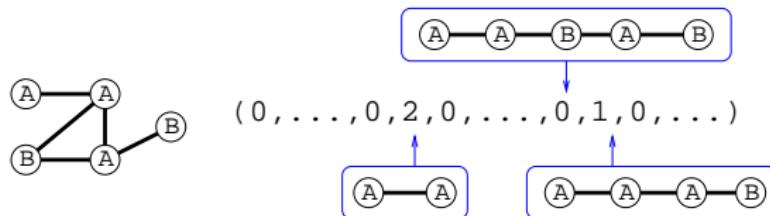
Indexing by specific subgraphs

Substructure selection

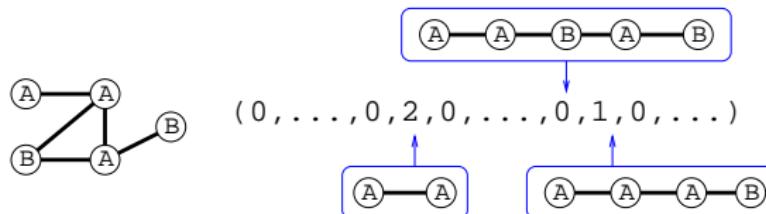
We can imagine more limited sets of substructures that lead to more computationnally efficient indexing (non-exhaustive list)

- substructures selected by **domain knowledge** (MDL fingerprint)
- all path **up to length k** (Openeye fingerprint, Nicholls 2005)
- all **shortest paths** (Borgwardt and Kriegel, 2005)
- all subgraphs **up to k vertices** (graphlet kernel, Sherashidze et al., 2009)
- all **frequent** subgraphs in the database (Helma et al., 2004)

Example : Indexing by all shortest paths



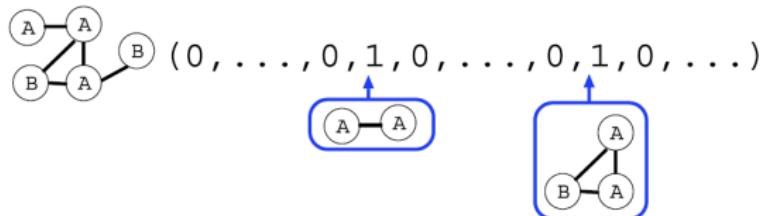
Example : Indexing by all shortest paths



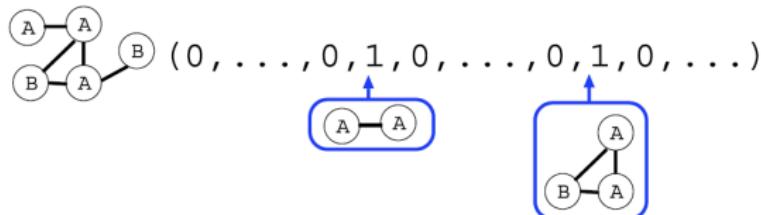
Properties (Borgwardt and Kriegel, 2005)

- There are $O(n^2)$ shortest paths.
- The vector of counts can be computed in $O(n^4)$ with the Floyd-Warshall algorithm.

Example : Indexing by all subgraphs up to k vertices



Example : Indexing by all subgraphs up to k vertices



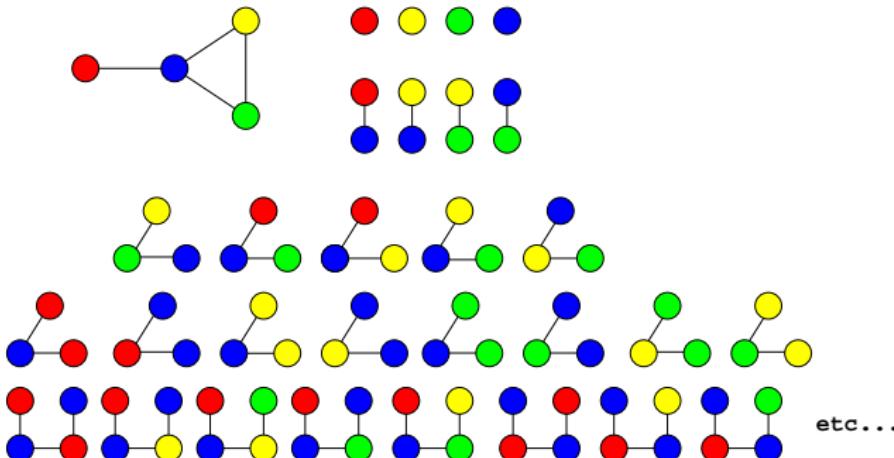
Properties (Shervashidze et al., 2009)

- Naive enumeration scales as $O(n^k)$.
- Enumeration of connected graphlets in $O(nd^{k-1})$ for graphs with degree $\leq d$ and $k \leq 5$.
- Randomly sample subgraphs if enumeration is infeasible.

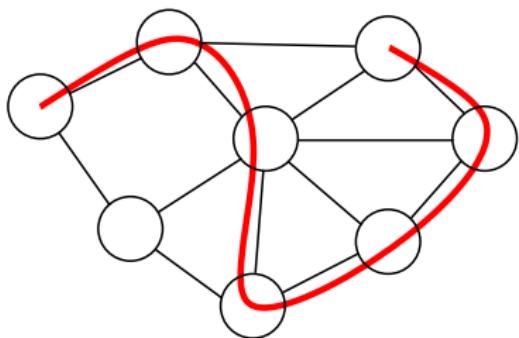
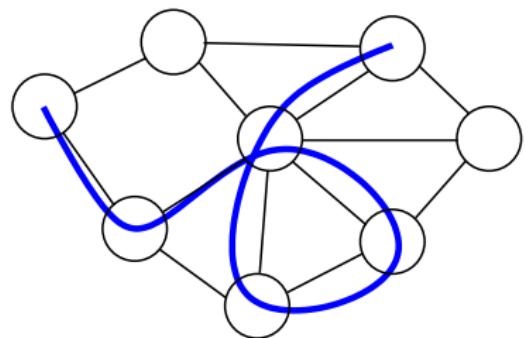
Walks

Definition

- A **walk** of a graph (V, E) is sequence of $v_1, \dots, v_n \in V$ such that $(v_i, v_{i+1}) \in E$ for $i = 1, \dots, n - 1$.
- We note $\mathcal{W}_n(G)$ the set of walks with n vertices of the graph G , and $\mathcal{W}(G)$ the set of all walks.



Walks \neq paths



Walk kernel

Definition

- Let \mathcal{S}_n denote the set of all possible **label sequences** of walks of length n (including vertices and edges labels), and $\mathcal{S} = \cup_{n \geq 1} \mathcal{S}_n$.
- For any graph \mathcal{X} let a **weight** $\lambda_G(w)$ be associated to each walk $w \in \mathcal{W}(G)$.
- Let the feature vector $\Phi(G) = (\Phi_s(G))_{s \in \mathcal{S}}$ be defined by:

$$\Phi_s(G) = \sum_{w \in \mathcal{W}(G)} \lambda_G(w) \mathbf{1} (s \text{ is the label sequence of } w).$$

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- A walk kernel is a graph kernel defined by:

$$K_{\text{walk}}(G_1, G_2) = \sum_{s \in \mathcal{S}} \Phi_s(G_1) \Phi_s(G_2).$$

Walk kernel examples

- The n th-order walk kernel is the walk kernel with $\lambda_G(w) = 1$ if the length of w is n , 0 otherwise. It compares two graphs through their common walks of length n .

Walk kernel examples

- The *n*th-order walk kernel is the walk kernel with $\lambda_G(w) = 1$ if the length of w is n , 0 otherwise. It compares two graphs through their common walks of length n .
- The random walk kernel is obtained with $\lambda_G(w) = P_G(w)$, where P_G is a Markov random walk on G . In that case we have:

$$K(G_1, G_2) = P(\text{label}(W_1) = \text{label}(W_2)),$$

where W_1 and W_2 are two independant random walks on G_1 and G_2 , respectively (Kashima et al., 2003).

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- The geometric walk kernel is obtained (when it converges) with $\lambda_G(w) = \beta^{\text{length}(w)}$, for $\beta > 0$. In that case the feature space is of infinite dimension (Gärtner et al., 2003).

Computation of walk kernels

Proposition

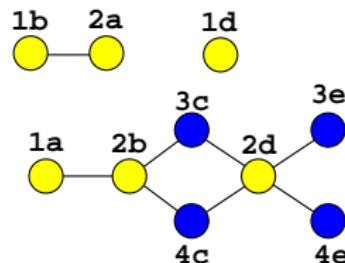
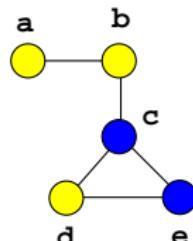
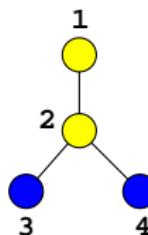
These three kernels (n th-order, random and geometric walk kernels) can be computed efficiently in **polynomial time**.

Product graph

Definition

Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two graphs with labeled vertices. The **product graph** $G = G_1 \times G_2$ is the graph $G = (V, E)$ with:

- ① $V = \{(v_1, v_2) \in V_1 \times V_2 : v_1 \text{ and } v_2 \text{ have the same label}\}$,
- ② $E = \{((v_1, v_2), (v'_1, v'_2)) \in V \times V : (v_1, v'_1) \in E_1 \text{ and } (v_2, v'_2) \in E_2\}.$



G_1

G_2

$G_1 \times G_2$

Walk kernel and product graph

Lemma

There is a **bijection** between:

- ① The **pairs of walks** $w_1 \in \mathcal{W}_n(G_1)$ and $w_2 \in \mathcal{W}_n(G_2)$ with the **same label sequences**,
- ② The **walks on the product graph** $w \in \mathcal{W}_n(G_1 \times G_2)$.

Walk kernel and product graph

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- ② The **walks on the product graph** $w \in \mathcal{W}_n(G_1 \times G_2)$.

Corollary

$$\begin{aligned} K_{\text{walk}}(G_1, G_2) &= \sum_{s \in \mathcal{S}} \Phi_s(G_1) \Phi_s(G_2) \\ &= \sum_{(w_1, w_2) \in \mathcal{W}(G_1) \times \mathcal{W}(G_2)} \lambda_{G_1}(w_1) \lambda_{G_2}(w_2) \mathbf{1}(l(w_1) = l(w_2)) \\ &= \sum_{w \in \mathcal{W}(G_1 \times G_2)} \lambda_{G_1 \times G_2}(w). \end{aligned}$$

Computation of the n th-order walk kernel

- For the n th-order walk kernel we have $\lambda_{G_1 \times G_2}(w) = 1$ if the length of w is n , 0 otherwise.
- Therefore:

$$K_{n\text{th-order}}(G_1, G_2) = \sum_{w \in \mathcal{W}_n(G_1 \times G_2)} 1.$$

- Let A be the adjacency matrix of $G_1 \times G_2$. Then we get:

$$K_{n\text{th-order}}(G_1, G_2) = \sum_{i,j} [A^n]_{i,j} = \mathbf{1}^\top A^n \mathbf{1}.$$

- Computation in $O(n|G_1||G_2|d_1 d_2)$, where d_i is the maximum degree of G_i .

Computation of random and geometric walk kernels

- In both cases $\lambda_G(w)$ for a walk $w = v_1 \dots v_n$ can be decomposed as:

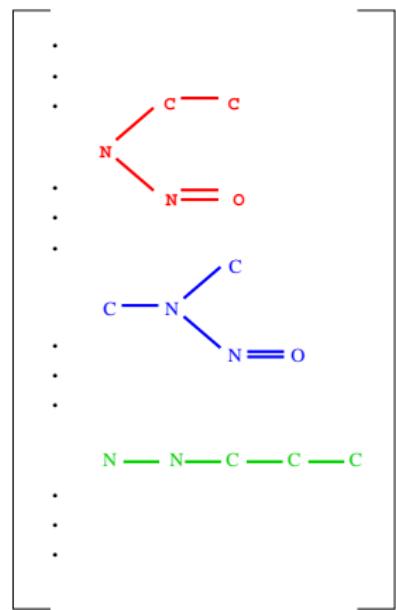
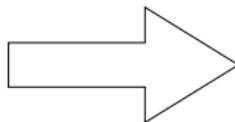
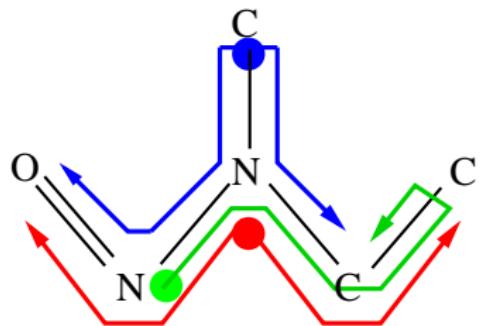
$$\lambda_G(v_1 \dots v_n) = \lambda^i(v_1) \prod_{i=2}^n \lambda^t(v_{i-1}, v_i).$$

- Let Λ_i be the vector of $\lambda^i(v)$ and Λ_t be the matrix of $\lambda^t(v, v')$:

$$\begin{aligned} K_{\text{walk}}(G_1, G_2) &= \sum_{n=1}^{\infty} \sum_{w \in \mathcal{W}_n(G_1 \times G_2)} \lambda^i(v_1) \prod_{i=2}^n \lambda^t(v_{i-1}, v_i) \\ &= \sum_{n=0}^{\infty} \Lambda_i \Lambda_t^n \mathbf{1} \\ &= \color{red} \Lambda_i (I - \Lambda_t)^{-1} \mathbf{1} \end{aligned}$$

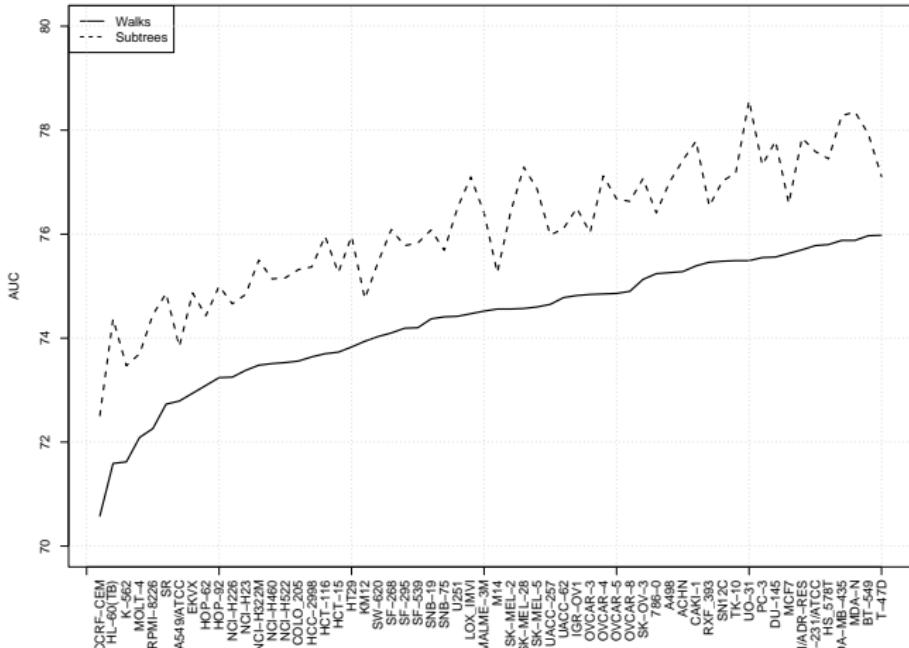
- Computation in $O(|G_1|^3 |G_2|^3)$

Extension: branching walks (Ramon and Gärtner, 2003; Mahé and Vert, 2009)



$$\mathcal{T}(v, n+1) = \sum_{R \subset \mathcal{N}(v)} \prod_{v' \in R} \lambda_t(v, v') \mathcal{T}(v', n),$$

2D Subtree vs walk kernels

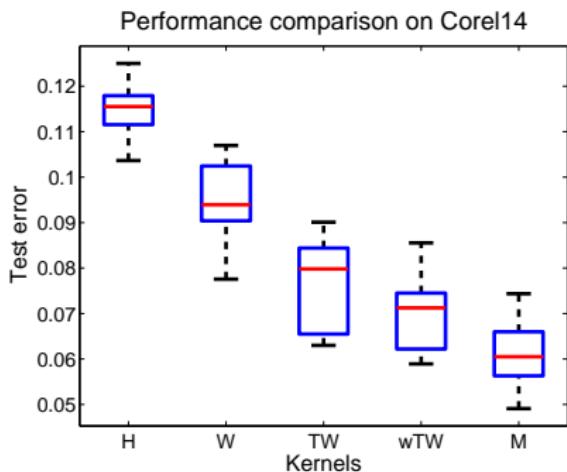


Screening of inhibitors for 60 cancer cell lines.

Image classification (Harchaoui and Bach, 2007)

COREL14 dataset

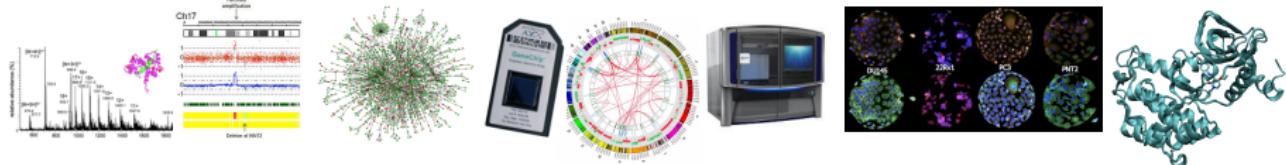
- 1400 natural images in 14 classes
- Compare kernel between histograms (H), walk kernel (W), subtree kernel (TW), weighted subtree kernel (wTW), and a combination (M).



Outline

- 1 Learning in high dimension
- 2 Learning with ℓ_2 regularization
 - Ridge regression
 - Ridge logistic regression
 - Linear hard-margin SVM
 - Interlude: quick notes on constrained optimization
 - Back to hard-margin SVM
 - Soft-margin SVM
 - Large-margin classifiers
- 3 Learning with kernels
 - Kernel methods
 - Positive definite kernels and RKHS
 - Kernel examples
 - Multiple Kernel Learning (MKL)
- 4 Conclusion

Motivation



- We have seen how to make learning algorithms given a kernel K on some data space \mathcal{X}
- Often we may have **several possible kernels**:
 - by **varying the kernel type or parameters** on a given description of the data (eg, linear, polynomial, Gaussian kernels with different bandwidths...)
 - because we have **different views of the same data**, eg, a protein can be characterized by its sequence, its structure, its mass spectrometry profile...
- How to **choose or integrate** different kernels in a learning task?

Setting: learning with one kernel

- For any $f : \mathcal{X} \rightarrow \mathbb{R}$, let $f^n = (f(x_1), \dots, f(x_n)) \in \mathbb{R}^n$
- Given a p.d. kernel $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$, we learn with K by solving:

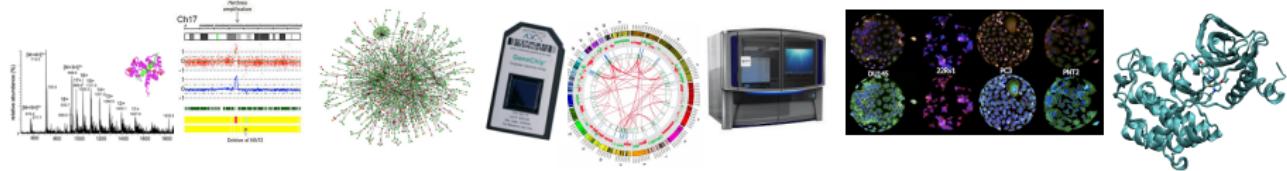
$$\min_{f \in \mathcal{H}} R(f^n) + \lambda \|f\|_{\mathcal{H}}^2, \quad (2)$$

where $\lambda > 0$ and $R : \mathbb{R}^n \rightarrow \mathbb{R}$ is an **closed**¹ and **convex** empirical risk:

- $R(u) = \frac{1}{n} \sum_{i=1}^n (u_i - y_i)^2$ for kernel ridge regression
- $R(u) = \frac{1}{n} \sum_{i=1}^n \max(1 - y_i u_i, 0)$ for SVM
- $R(u) = \frac{1}{n} \sum_{i=1}^n \log(1 + \exp(-y_i u_i))$ for kernel logistic regression

¹ R is closed if, for each $A \in \mathbb{R}$, the sublevel set $\{u \in \mathbb{R}^n : R(u) \leq A\}$ is closed. For example, if R is continuous then it is closed.

Sum kernel



Definition

Let K_1, \dots, K_M be M kernels on \mathcal{X} . The sum kernel K_S is the kernel on \mathcal{X} defined as

$$\forall x, x' \in \mathcal{X}, \quad K_S(x, x') = \sum_{i=1}^M K_i(x, x').$$

Sum kernel and vector concatenation

Theorem

For $i = 1, \dots, M$, let $\Phi_i : \mathcal{X} \rightarrow \mathcal{H}_i$ be a feature map such that

$$K_i(x, x') = \langle \Phi_i(x), \Phi_i(x') \rangle_{\mathcal{H}_i}.$$

Then $K_S = \sum_{i=1}^M K_i$ can be written as:

$$K_S(x, x') = \langle \Phi_S(x), \Phi_S(x') \rangle_{\mathcal{H}_S},$$

where $\Phi_S : \mathcal{X} \rightarrow \mathcal{H}_S = \mathcal{H}_1 \oplus \dots \oplus \mathcal{H}_M$ is the **concatenation** of the feature maps Φ_i :

$$\Phi_S(x) = (\Phi_1(x), \dots, \Phi_M(x))^\top.$$

Therefore, summing kernels amounts to concatenating their feature space representations, which is a quite natural way to integrate different features.

Proof

For $\Phi_S(x) = (\Phi_1(x), \dots, \Phi_M(x))^\top$, we easily compute:

$$\begin{aligned}\langle \Phi_S(x), \Phi_S(x') \rangle_{\mathcal{H}_S} &= \sum_{i=1}^M \langle \Phi_i(x), \Phi_i(x') \rangle_{\mathcal{H}_i} \\ &= \sum_{i=1}^M K_i(x, x') \\ &= K_S(x, x').\end{aligned}$$

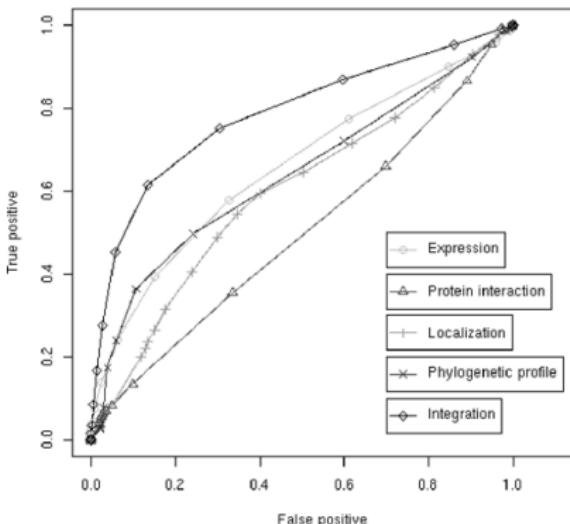
Example: data integration with the sum kernel



Protein network inference from multiple genomic data: a supervised approach

Y. Yamanishi^{1,*}, J.-P. Vert² and M. Kanehisa¹

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K_{exp} (Expression)

K_{ppi} (Protein interaction)

K_{loc} (Localization)

K_{phy} (Phylogenetic profile)

$K_{\text{exp}} + K_{\text{ppi}} + K_{\text{loc}} + K_{\text{phy}}$
(Integration)

The sum kernel: functional point of view

Theorem

The solution $f^* \in \mathcal{H}_{K_S}$ when we learn with $K_S = \sum_{i=1}^M K_i$ is equal to:

$$f^* = \sum_{i=1}^M f_i^*,$$

where $(f_1^*, \dots, f_M^*) \in \mathcal{H}_{K_1} \times \dots \times \mathcal{H}_{K_M}$ is the solution of:

$$\min_{f_1, \dots, f_M} R \left(\sum_{i=1}^M f_i^n \right) + \lambda \sum_{i=1}^M \| f_i \|_{\mathcal{H}_{K_i}}^2.$$

Generalization: The weighted sum kernel

Theorem

The solution f^* when we learn with $K_\eta = \sum_{i=1}^M \eta_i K_i$, with $\eta_1, \dots, \eta_M \geq 0$, is equal to:

$$f^* = \sum_{i=1}^M f_i^*,$$

where $(f_1^*, \dots, f_M^*) \in \mathcal{H}_{K_1} \times \dots \times \mathcal{H}_{K_M}$ is the solution of:

$$\min_{f_1, \dots, f_M} R \left(\sum_{i=1}^M f_i^n \right) + \lambda \sum_{i=1}^M \frac{\| f_i \|_{\mathcal{H}_{K_i}}^2}{\eta_i}.$$

Proof (1/4)

$$\min_{f_1, \dots, f_M} R \left(\sum_{i=1}^M f_i^n \right) + \lambda \sum_{i=1}^M \frac{\| f_i \|_{\mathcal{H}_{K_i}}^2}{\eta_i}.$$

- R being convex, the problem is strictly convex and has a **unique solution** $(f_1^*, \dots, f_M^*) \in \mathcal{H}_{K_1} \times \dots \times \mathcal{H}_{K_M}$.
- By the representer theorem, there exists $\alpha_1^*, \dots, \alpha_M^* \in \mathbb{R}^n$ such that

$$f_i^*(x) = \sum_{j=1}^n \alpha_{ij}^* K_i(x_j, x).$$

- $(\alpha_1^*, \dots, \alpha_M^*)$ is the solution of

$$\min_{\alpha_1, \dots, \alpha_M \in \mathbb{R}^n} R \left(\sum_{i=1}^M K_i \alpha_i \right) + \lambda \sum_{i=1}^M \frac{\alpha_i^\top K_i \alpha_i}{\eta_i}.$$

Proof (2/4)

- This is equivalent to

$$\min_{u, \alpha_1, \dots, \alpha_M \in \mathbb{R}^n} R(u) + \lambda \sum_{i=1}^M \frac{\alpha_i^\top K_i \alpha_i}{\eta_i} \quad \text{s.t.} \quad u = \sum_{i=1}^M K_i \alpha_i.$$

- This is equivalent to the saddle point problem:

$$\min_{u, \alpha_1, \dots, \alpha_M \in \mathbb{R}^n} \max_{\gamma \in \mathbb{R}^n} R(u) + \lambda \sum_{i=1}^M \frac{\alpha_i^\top K_i \alpha_i}{\eta_i} + 2\lambda \gamma^\top (u - \sum_{i=1}^M K_i \alpha_i).$$

- By Slater's condition, strong duality holds, meaning we can invert min and max:

$$\max_{\gamma \in \mathbb{R}^n} \min_{u, \alpha_1, \dots, \alpha_M \in \mathbb{R}^n} R(u) + \lambda \sum_{i=1}^M \frac{\alpha_i^\top K_i \alpha_i}{\eta_i} + 2\lambda \gamma^\top (u - \sum_{i=1}^M K_i \alpha_i).$$

Proof (3/4)

- Minimization in u :

$$\min_u R(u) + 2\lambda\gamma^\top u = - \max_u \left\{ -2\lambda\gamma^\top u - R(u) \right\} = -R^*(-2\lambda\gamma),$$

where R^* is the Fenchel dual of R :

$$\forall v \in \mathbb{R}^n \quad R^*(v) = \sup_{u \in \mathbb{R}^n} u^\top v - R(u).$$

- Minimization in α_i for $i = 1, \dots, M$:

$$\min_{\alpha_i} \left\{ \lambda \frac{\alpha_i^\top K_i \alpha_i}{\eta_i} - 2\lambda\gamma^\top K_i \alpha_i \right\} = -\lambda\eta_i\gamma^\top K_i\gamma,$$

where the minimum in α_i is reached for $\alpha_i^* = \eta_i\gamma$.

Proof (4/4)

- The dual problem is therefore

$$\max_{\gamma \in \mathbb{R}^n} \left\{ -R^*(-2\lambda\gamma) - \lambda\gamma^\top \left(\sum_{i=1}^M \eta_i K_i \right) \gamma \right\}.$$

- Note that if learn from a single kernel K_η , we get the same dual problem

$$\max_{\gamma \in \mathbb{R}^n} \left\{ -R^*(-2\lambda\gamma) - \lambda\gamma^\top K_\eta \gamma \right\}.$$

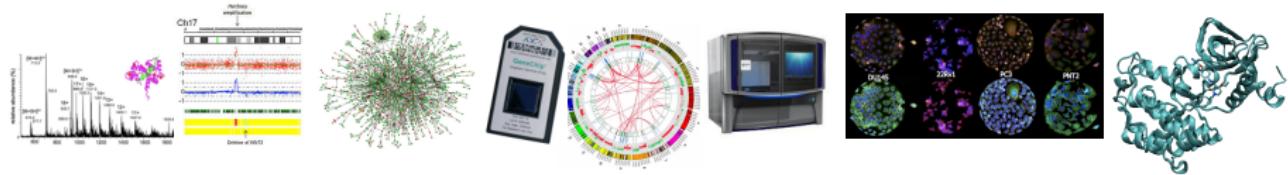
- If γ^* is a solution of the dual problem, then $\alpha_i^* = \eta_i \gamma^*$ leading to:

$$\forall x \in \mathcal{X}, \quad f_i^*(x) = \sum_{j=1}^n \alpha_{ij}^* K_i(x_j, x) = \sum_{j=1}^n \eta_i \gamma_j^* K_i(x_j, x)$$

- Therefore, $f^* = \sum_{i=1}^M f_i^*$ satisfies

$$f^*(x) = \sum_{i=1}^M \sum_{j=1}^n \eta_i \gamma_j^* K_i(x_j, x) = \sum_{j=1}^n \gamma_j^* K_\eta(x_j, x). \quad \square$$

Learning the kernel



Motivation

- If we know how to weight each kernel, then we can learn with the weighted kernel

$$K_\eta = \sum_{i=1}^M \eta_i K_i$$

- However, usually we don't know...
- Perhaps we can optimize the weights η_i during learning?

An objective function for K

Theorem

For any p.d. kernel K on \mathcal{X} , let

$$J(K) = \min_{f \in \mathcal{H}} \{ R(f^n) + \lambda \| f \|_{\mathcal{H}}^2 \} .$$

The function $K \mapsto J(K)$ is **convex**.

This suggests a principled way to "learn" a kernel: define a convex set of candidate kernels, and minimize $J(K)$ by convex optimization.

Proof

- We have shown by strong duality that

$$J(K) = \max_{\gamma \in \mathbb{R}^n} \left\{ -R^*(-2\lambda\gamma) - \lambda\gamma^\top K\gamma \right\}.$$

- For each γ fixed, this is an affine function of K , hence convex
- A supremum of convex functions is convex. □

□

MKL (Lanckriet et al., 2004)

- We consider the set of **convex combinations**

$$K_\eta = \sum_{i=1}^M \eta_i K_i \quad \text{with} \quad \eta \in \Sigma_M = \left\{ \eta_i \geq 0, \sum_{i=1}^M \eta_i = 1 \right\}$$

- We optimize both η and f^* by solving:

$$\min_{\eta \in \Sigma_M} J(K_\eta) = \min_{\eta \in \Sigma_M} \min_{f \in \mathcal{H}_{K_\eta}} \left\{ R(f^n) + \lambda \| f \|_{\mathcal{H}_{K_\eta}}^2 \right\}$$

- The problem is **jointly convex** in (η, α) and can be solved efficiently.
- The output is both a set of weights η , and a predictor corresponding to the kernel method trained with kernel K_η .
- This method is usually called **Multiple Kernel Learning (MKL)**.

Example: protein annotation



A statistical framework for genomic data fusion

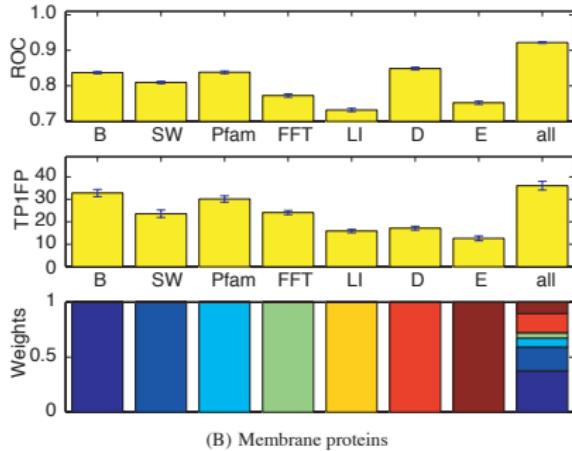
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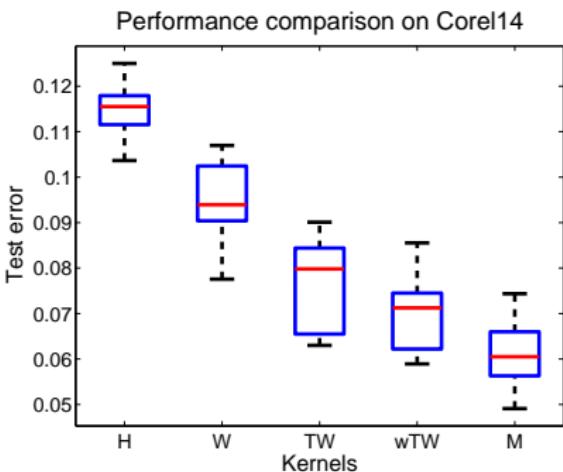


Kernel	Data	Similarity measure
K_{SW}	protein sequences	Smith-Waterman
K_B	protein sequences	BLAST
K_{Pfam}	protein sequences	Pfam HMM
K_{FFT}	hydropathy profile	FFT
K_{LI}	protein interactions	linear kernel
K_D	protein interactions	diffusion kernel
K_E	gene expression	radial basis kernel
K_{RND}	random numbers	linear kernel

Example: Image classification (Harchaoui and Bach, 2007)

COREL14 dataset

- 1400 natural images in 14 classes
- Compare kernel between histograms (H), walk kernel (W), subtree kernel (TW), weighted subtree kernel (wTW), and a combination by MKL (M).



MKL revisited (Bach et al., 2004)

$$K_\eta = \sum_{i=1}^M \eta_i K_i \quad \text{with} \quad \eta \in \Sigma_M = \left\{ \eta_i \geq 0, \sum_{i=1}^M \eta_i = 1 \right\}$$

Theorem

The solution f^* of

$$\min_{\eta \in \Sigma_M} \min_{f \in \mathcal{H}_{K_\eta}} \left\{ R(f^n) + \lambda \| f \|_{\mathcal{H}_{K_\eta}}^2 \right\}$$

is $f^* = \sum_{i=1}^M f_i^*$, where $(f_1^*, \dots, f_M^*) \in \mathcal{H}_{K_1} \times \dots \times \mathcal{H}_{K_M}$ is the solution of:

$$\min_{f_1, \dots, f_M} \left\{ R \left(\sum_{i=1}^M f_i^n \right) + \lambda \left(\sum_{i=1}^M \| f_i \|_{\mathcal{H}_{K_i}} \right)^2 \right\}.$$

Proof (1/2)

$$\begin{aligned} & \min_{\eta \in \Sigma_M} \min_{f \in \mathcal{H}_{K_\eta}} \left\{ R(f^n) + \lambda \| f \|_{\mathcal{H}_{K_\eta}}^2 \right\} \\ &= \min_{\eta \in \Sigma_M} \min_{f_1, \dots, f_M} \left\{ R \left(\sum_{i=1}^M f_i^n \right) + \lambda \sum_{i=1}^M \frac{\| f_i \|_{\mathcal{H}_{K_i}}^2}{\eta_i} \right\} \\ &= \min_{f_1, \dots, f_M} \left\{ R \left(\sum_{i=1}^M f_i^n \right) + \lambda \min_{\eta \in \Sigma_M} \left\{ \sum_{i=1}^M \frac{\| f_i \|_{\mathcal{H}_{K_i}}^2}{\eta_i} \right\} \right\} \\ &= \min_{f_1, \dots, f_M} \left\{ R \left(\sum_{i=1}^M f_i^n \right) + \lambda \left(\sum_{i=1}^M \| f_i \|_{\mathcal{H}_{K_i}} \right)^2 \right\}, \end{aligned}$$

Proof (2/2)

where the last equality results from:

$$\forall \mathbf{a} \in \mathbb{R}_+^M, \quad \left(\sum_{i=1}^M a_i \right)^2 = \inf_{\eta \in \Sigma_M} \sum_{i=1}^M \frac{a_i^2}{\eta_i},$$

which is a direct consequence of the Cauchy-Schwarz inequality:

$$\sum_{i=1}^M a_i = \sum_{i=1}^M \frac{a_i}{\sqrt{\eta_i}} \times \sqrt{\eta_i} \leq \left(\sum_{i=1}^M \frac{a_i^2}{\eta_i} \right)^{\frac{1}{2}} \left(\sum_{i=1}^M \eta_i \right)^{\frac{1}{2}}.$$

Algorithm: simpleMKL (Rakotomamonjy et al., 2008)

- We want to minimize in $\eta \in \Sigma_M$:

$$\min_{\eta \in \Sigma_M} J(K_\eta) = \min_{\eta \in \Sigma_M} \max_{\gamma \in \mathbb{R}^n} \left\{ -R^*(-2\lambda\gamma) - \lambda\gamma^\top K_\eta \gamma \right\}.$$

- For a fixed $\eta \in \Sigma_M$, we can compute $f(\eta) = J(K_\eta)$ by using a standard solver for a single kernel to find γ^* :

$$J(K_\eta) = -R^*(-2\lambda\gamma^*) - \lambda\gamma^{*\top} K_\eta \gamma^*.$$

- From γ^* we can also compute the gradient of $J(K_\eta)$ with respect to η :

$$\frac{\partial J(K_\eta)}{\partial \eta_i} = -\lambda\gamma^{*\top} K_i \gamma^*.$$

- $J(K_\eta)$ can then be minimized on Σ_M by a projected gradient or reduced gradient algorithm.

Sum kernel vs MKL

- Learning with the sum kernel (uniform combination) solves

$$\min_{f_1, \dots, f_M} \left\{ R \left(\sum_{i=1}^M f_i^n \right) + \lambda \sum_{i=1}^M \| f_i \|_{\mathcal{H}_{K_i}}^2 \right\}.$$

- Learning with MKL (best convex combination) solves

$$\min_{f_1, \dots, f_M} \left\{ R \left(\sum_{i=1}^M f_i^n \right) + \lambda \left(\sum_{i=1}^M \| f_i \|_{\mathcal{H}_{K_i}} \right)^2 \right\}.$$

- Although MKL can be thought of as optimizing a convex combination of kernels, it is more correct to think of it as a penalized risk minimization estimator with the **group lasso** penalty:

$$\Omega(f) = \min_{f_1 + \dots + f_M = f} \sum_{i=1}^M \| f_i \|_{\mathcal{H}_{K_i}}.$$

Example: ridge vs LASSO regression

- Take $\mathcal{X} = \mathbb{R}^d$, and for $x = (x_1, \dots, x_d)^\top$ consider the **rank-1 kernels**:

$$\forall i = 1, \dots, d, \quad K_i(x, x') = x_i x'_i.$$

- A function $f_i \in \mathcal{H}_{K_i}$ has the form $f_i(x) = \beta_i x_i$, with $\|f_i\|_{\mathcal{H}_{K_i}} = |\beta_i|$.
- The sum kernel is $K_S(x, x') = \sum_{i=1}^d x_i x'_i = x^\top x$, a function \mathcal{H}_{K_S} is of the form $f(x) = \boldsymbol{\beta}^\top x$, with norm $\|f\|_{\mathcal{H}_{K_S}} = \|\boldsymbol{\beta}\|_{\mathbb{R}^d}$.
- Learning with the **sum kernel** solves a **ridge regression** problem:

$$\min_{\boldsymbol{\beta} \in \mathbb{R}^d} \left\{ R(X\boldsymbol{\beta}) + \lambda \sum_{i=1}^d \beta_i^2 \right\}.$$

- Learning with **MKL** solves a **LASSO regression** problem:

$$\min_{\boldsymbol{\beta} \in \mathbb{R}^d} \left\{ R(X\boldsymbol{\beta}) + \lambda \left(\sum_{i=1}^d |\beta_i| \right)^2 \right\}.$$

Extensions (Micchelli et al., 2005)

For $r > 0$, $K_\eta = \sum_{i=1}^M \eta_i K_i$ with $\eta \in \Sigma_M^r = \left\{ \eta_i \geq 0, \sum_{i=1}^M \eta_i^r = 1 \right\}$

Theorem

The solution f^* of

$$\min_{\eta \in \Sigma_M^r} \min_{f \in \mathcal{H}_{K_\eta}} \left\{ R(f^n) + \lambda \|f\|_{\mathcal{H}_{K_\eta}}^2 \right\}$$

is $f^* = \sum_{i=1}^M f_i^*$, where $(f_1^*, \dots, f_M^*) \in \mathcal{H}_{K_1} \times \dots \times \mathcal{H}_{K_M}$ is the solution of:

$$\min_{f_1, \dots, f_M} \left\{ R \left(\sum_{i=1}^M f_i^n \right) + \lambda \left(\sum_{i=1}^M \|f_i\|_{\mathcal{H}_{K_i}}^{\frac{2r}{r+1}} \right)^{\frac{r+1}{r}} \right\}.$$

Outline

- 1 Learning in high dimension
- 2 Learning with ℓ_2 regularization
 - Ridge regression
 - Ridge logistic regression
 - Linear hard-margin SVM
 - Interlude: quick notes on constrained optimization
 - Back to hard-margin SVM
 - Soft-margin SVM
 - Large-margin classifiers
- 3 Learning with kernels
 - Kernel methods
 - Positive definite kernels and RKHS
 - Kernel examples
 - Multiple Kernel Learning (MKL)
- 4 Conclusion

In one slide...

- Learning in high dimension requires regularization, e.g., by ℓ_2 penalty for linear methods
- Kernels allow to transform any ℓ_2 -regularized linear models into a nonlinear model, thanks to the kernel trick
- There exists many kernels, which correspond to different feature spaces (of finite or infinite dimensions)
- We can combine and learn kernels, e.g., for integration of heterogeneous data
- Hot research topics
 - Large-scale ML with kernels
 - Deep kernel methods

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MURAKOZE

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